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Columbus

FILE 'HOME' ENTERED AT 18:38:39 ON 11 AUG 2005

\* \* STN

=> fil reg COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 0.21 0.21

FULL ESTIMATED COST

FILE 'REGISTRY' ENTERED AT 18:38:47 ON 11 AUG 2005 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2005 American Chemical Society (ACS)

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STRUCTURE FILE UPDATES: HIGHEST RN 859511-21-0 10 AUG 2005 DICTIONARY FILE UPDATES: 10 AUG 2005 HIGHEST RN 859511-21-0

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

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\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* \* The CA roles and document type information have been removed from \* the IDE default display format and the ED field has been added, \* effective March 20, 2005. A new display format, IDERL, is now \* available and contains the CA role and document type information. \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

Structure search iteration limits have been increased. See HELP SLIMITS for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at: http://www.cas.org/ONLINE/DBSS/registryss.html

Uploading C:\Program Files\Stnexp\Queries\10784916\10784916d.str

chain nodes:
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 18 19
chain bonds:
1-2 2-3 2-18 3-4 4-5 5-6 6-7 6-8 8-9 9-10 10-11 10-12 12-13 13-14
14-15 14-16 14-19

exact/norm bonds:
1-2 2-3 2-18 3-4 4-5 5-6 6-7 6-8 8-9 9-10 10-11 10-12 12-13 13-14
14-15 14-16 14-19

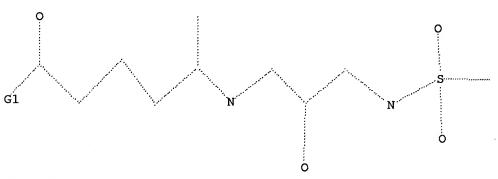
G1:C,O,N

Match level:

1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 18:CLASS 19:CLASS

# L1 STRUCTURE UPLOADED

=> d L1 HAS NO ANSWERS L1 STR



G1 C, O, N

Structure attributes must be viewed using STN Express query preparation.

=> s L1
SAMPLE SEARCH INITIATED 18:39:12 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 17 TO ITERATE

100.0% PROCESSED 17 ITERATIONS 0 ANSWERS SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 93 TO 587
PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> s L1 full

FULL SEARCH INITIATED 18:39:17 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 437 TO ITERATE

100.0% PROCESSED 437 ITERATIONS 0 ANSWERS

SEARCH TIME: 00.00.01

L3 0 SEA SSS FUL L1

=> fil reg

COST IN U.S. DOLLARS SINCE FILE TOTAL

FULL ESTIMATED COST ENTRY SESSION 162.19 162.40

FILE 'REGISTRY' ENTERED AT 18:40:27 ON 11 AUG 2005 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2005 American Chemical Society (ACS)

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STRUCTURE FILE UPDATES: 10 AUG 2005 HIGHEST RN 859511-21-0 DICTIONARY FILE UPDATES: 10 AUG 2005 HIGHEST RN 859511-21-0

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Structure search iteration limits have been increased. See HELP SLIMITS for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at: http://www.cas.org/ONLINE/DBSS/registryss.html

=>

Uploading C:\Program Files\Stnexp\Queries\10784916\10784916e.str

chain nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 18

ring/chain nodes :

19

chain bonds :

 $1-2 \quad 2-3 \quad 2-18 \quad 3-4 \quad 4-5 \quad 5-6 \quad 6-7 \quad 6-8 \quad 8-9 \quad 9-10 \quad 10-11 \quad 10-12 \quad 12-13 \quad 13-14$ 

14-15 14-16 14-19 exact/norm bonds:

1-2 2-3 2-18 3-4 4-5 5-6 6-7 6-8 8-9 9-10 10-11 10-12 12-13 13-14

14-15 14-16 14-19

G1:C,O,N

Match level:

1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 18:CLASS 19:CLASS

# L4 STRUCTURE UPLOADED

=> d

L4 HAS NO ANSWERS

L4 STR

G1 C, O, N

Structure attributes must be viewed using STN Express query preparation.

=> s L4

SAMPLE SEARCH INITIATED 18:40:56 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 56 TO ITERATE

100.0% PROCESSED

56 ITERATIONS

5 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS:

672 TO 1568

PROJECTED ANSWERS:

5 TO 234

L5

5 SEA SSS SAM L4

=> s L4 full

FULL SEARCH INITIATED 18:41:00 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 1291 TO ITERATE

100.0% PROCESSED 1291 ITERATIONS

110 ANSWERS

SEARCH TIME: 00.00.01

L6 110 SF

110 SEA SSS FUL L4

=> fil caplus

COST IN U.S. DOLLARS

SINCE FILE TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

161.33 323.73

FILE 'CAPLUS' ENTERED AT 18:41:04 ON 11 AUG 2005
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FILE COVERS 1907 - 11 Aug 2005 VOL 143 ISS 7 FILE LAST UPDATED: 10 Aug 2005 (20050810/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s L6

L7

19 L6

=> d ibib abs hitstr

L7 ANSWER 1 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER:
DOCUMENT NUMBER:
117LE:
117VENTOR(S):
1205:527407 CAPLUS
143:59982
Preparation of HIV protease inhibitors, in particular inidazolidine derivatives
Flentye, Charles A.; Chen, Hui-Ju; Degoey, David A.;
Plosi, William J., Grampovnik, David J.; Huang, Pegy
P.; Kempf, Dale J.; Klein, Larry L.; Krueger, Allan
C.; Madigan, Darold L.; Radolph, John T.; Sun,
Minghus; Yeung, Ming C.; Zhao, Chen
USA
SOURCE:
USA
U.S. Pat. Appl. Publ., 287 pp.
CODEN: USXKCO
DOCUMENT TYPE:
PANILY ACC. NUM. COUNT:
1

FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PATI	ENT I	NO.			KIN	D	DATE			APPL	ICAT	ION :	NO.		D.	ATE		
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			42		A1		2005									0031		
wo :	2005	0614	50		A2		2005	0707		¥0 2	004-	US37	745		2	0041	110	
	w:	ΑE,	λG,	AL,	λM,	AT,	AU,	AZ,	BA,	BB,	BG,	BR,	B₩,	BY,	BZ,	CA,	CH,	
		αi,	œ,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EK,	EG,	ËS,	FI,	GB,	GD,	
		GE,	GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	KP,	KR,	KZ,	LC,	
		LK,	LR,	LS,	LT,	w,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NA,	NI,	
		NO,	NZ.	ΟM,	PG,	PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	SY,	
		TJ,	TM,	TN,	TR,	TT,	TZ,	UA,	UG,	US,	UZ,	VC,	VN,	YU,	ZA,	ZM,	ZW	
	RV:	BW,	GH,	GM,	ΧŒ,	LS,	MV,	MZ,	NA,	SD,	SL,	SZ,	ΤZ,	UG,	ZM,	ZW,	AM,	
		ΑZ,	BY,	KG,	ĸz,	MD,	Rυ,	TJ,	TM,	AΤ,	BK,	BG,	ŒŦ,	CY,	CZ,	DE,	DK,	
		EE,	ES,	FI,	FR,	GB,	GR,	ΗU,	IE,	ıs,	IT,	LU,	MC,	NL,	PL,	PT,	RO,	
		SE,	SI,	SK,	TR,	BF,	ВJ,	CF,	œ,	CI,	CΜ,	GΑ,	GN,	GQ,	GW,	ML,	MR,	
		NE,	SN,	TD,	TG													
MORITY	APP	LN.	INFO	.:						US 2	003-	7339	15		A 2	0031	211	

## \* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

Title compds. of formula ANH(CHR)(CHR)(CHR))(CHR2)NR3S(O2)R4 (I) [wherein A = alkylcarbonyl, arylsulfonyl, 1,3-substituted 2-oxoimidazolidinyl, 2,4-dioxoimidazolidinyl, etc.; X, Y = independently O, S, NH; R = (un)substituted alk(en)yl, cycloalk(en)yl, hetero/arylalkyl, etc.; R1 = OH and derivs., 0703H and derivs., 0502H and derivs., etc.; R2 = H; R3 = halo/alkyl, halo/alkyl, halo/alkenyl, (un)substituted cycloalk(en)yl, aryl, R4 = (un)substituted cycloalk(en)yl, etc.; R2 = H; R3 = halo/alkyl, halo/alkenyl, un)substituted cycloalk(en)yl, ryl, R4 = (un)substituted cycloalk(en)yl, heterocyclyl, heterofaryl) were prepared as HIV protease inhibitors. For example, II was prepared, in 628 yield, by coupling acid III (preparation given) with amine IV (preparation given). I

antiviral activity against Wild-Type HIV with EC50 in the range of 1 nM to

100 nM. 854742-03-39 854742-719 854742-66-89 854742-66-09 854742-69-39 854742-719 854742-80-69 854746-70-69 854746-71-79 854746-72-89 RL: PAC (Pharmacological activity): SPN (Synthetic preparation): TRU (Therapeutic use): BIOL (Biological study): PREP (Preparation): USES (Uses)

es) (antiviral agent; preparation of HIV protease inhibitors, in particular imidazolidine derivs.)

ANSWER 1 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

 $854742-68-0 \quad CAPLUS \\ Pentanediant.de, N-{(1S,2R)-2-hydroxy-3-{[(4-methoxyphenyl)sulfonyl](2-methylpropyl)sulfon)-1-(phenylmethyl)propyl]-2-{3-{(2-methyl-4-thiazolyl)methyl}-2-oxo-1-imidazolidinyl]-, (2S)- {9CI} (CA INDEX NAMINGAR) (CA INDEX NAMINGAR)$ (CA INDEX NAME)

Absolute stereochemistry.

854742-79-3 CAPLUS Butanedlamide, N1-[(15,2R)-2-hydroxy-3-[[(4-methoxyphenyl) sulfonyl](2-methyl)-gropyl) amino]-1-(phenylmethyl)-gropyl]-N4-methyl-2-[3-[(2-methyl-4-thiazolyl)methyl)-2-oxo-1-imidazolidinyl]-, (25)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSVER 1 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN (Continued) 854742-03-3 CAPLUS Carbanic acid, {[15)-3-amino-1-[[{(15,2R)-2-hydroxy-3-[[4-[E)-(hydroxyiaino] mathyl]phenyl]sulfonyl]{2-methylpropyl}amino]-1-(phenylnethyl)propyl]amino]carbonyl]-3-oxopropyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

854742-27-1 CAPLUS INDEX NAME NOT YET ASSIGNED

Absolute stereochemistry. Double bond geometry as shown.

854742-66-8 CAPLUS Butanedianide, N1-[(15,2R)-2-hydroxy-3-[[(4-methoxyphenyl) sulfonyl] (2-methylpropyl) amino]-1-(phenylmethyl) propyl]-2-[3-[(2-methyl-4-thiazolyl)methyl]-2-oxo-1-imidazolidinyl]-, (25)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 1 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

854742-80-6 CAPLUS Butanediamide, N#-ethyl-N1-[(1S,2R)-2-hydroxy-3-[[(4-methynyl)sulfonyl](2-methylpropyl)amino]-1-[phenylmethyl)propyl]-2-[3-[(2-methyl-4-thiazolyl)methyl]-2-oxo-1-imidazolidinyl]-, (2S)- (9CI) (CA INDEX NAME)

854746-70-6 CAPLUS PentanediamIde, N5-[(15,2R)-2-hydroxy-3-[((4-methoxyphenyl) sulfonyl](2-methylpropyl) aminol-1-(phenylmethyl)propyl]-2-[3-[(2-methyl-4-thiazolyl)methyl]-2-oxo-l-imidazolidinyl]-, (25)- (9CI) (CA INDEX NAME)

RN 854746-71-7 CAPLUS
CN Butanedianide, N-[(15,2R)-2-hydroxy-3-[[(4-methoxyphenyl)sulfonyl](2-methylpropyl)anino]-1-(phenylmethyl)propyl)-N'-[(25)-2-[3-[(2-methyl-5-thiazolyl)methyl]-2-oxo-1-inidazolidinyl]-1-oxopropyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-B

RN 854746-72-8 CAPLUS
CN Butanediamide, N-[(15,2R)-2-hydroxy-3-[[(4-methoxyphenyl)sulfonyl](2-methylpropyl)amino]-1-(phenylmethyl)propyl]-N\*-[(25)-2-[3-[(2-methyl-5-thiazolyl)methyl]-2-oxo-1-imidazolidinyl]-1-oxobutyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-B

=> d ibib abs hitstr 2-19

L7 ANSWER 2 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN ACCESSION NUMBER: 2004:322087 CAPLUS DOCUMENT NUMBER: 140:399222 TITLE: BREED: 5----

140:399222
BREED: Generating Novel Inhibitors through
Hybridization of Known Ligands. Application to CDX2,
P38, and HIV Protease
Pierce, Albert C.; Ran, Govinda; Bemis, Guy W.
Vertex Pharmaceuticals, Cambridge, MA, 02139, USA
Journal of Medicinal Chemistry (2004), 47(11),
CODEN: JMCMAP. IESU. 2022 2022 CORPORATE SOURCE: SOURCE:

2768-2775 CODEN: JMCMAR; ISSN: 0022-2623 American Chemical Society PUBLISHER: DOCUMENT TYPE:

Journal LANGUAGE:

NAME: English
In this work we describe BREED, a method for the generation of novel
inhibitors from structures of known ligands bound to a common target,
method is essentially an automation of the common medicinal chemical

method is essentially an automation of the common medicinal chemical rice
of joining fragments of two known ligands to generate a new inhibitor. The ligand-bound target structures are overlaid, all overlapping bonds in all pairs of ligands are found, and the fragments on each side of each matching bond are swapped to generate the new mols. Since the method is automated, it can be applied recursively to generate all possible combinations of known ligands. In an application of this method to HIV protease inhibitors and protein kinase inhibitors hundreds of new mol. structures were generated. These included known inhibitor scaffolds not included in the initial set, entirely novel scaffolds, and novel substituents on known scaffolds. The method is fast, and since all of the ligand functional groups are known to bind the target in the precise position and orientation present in the novel ligand, the success rate of this method should be superior to more traditional de novo design techniques. In an era of increasingly high-throughput structural biol., such methods for high-throughput utilization of structural information will become increasingly valuable.

688359-10-6

RL-SSU (Biological study, unclassified), BIOL (Biological study)

688359-10-6
RI: BSU (Biological study, unclassified), BIOL (Biological study)
(novel method BREED for generating novel inhibitors through
bond-matching and fragment swapping of known ligands)
688359-10-6 CAPLUS
Butanediamide, N1-{(15,2R)-3-[(4-aminophenyl)sulfonyl](2methylpropyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-2-((2quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

REFERENCE COUNT:

THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7- ANSWER 3 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN W 1994-US9139 US 1995-251090 US 1999-288080 US 1999-288080

W 19940823 A3 19950525 A1 19990408 US 2002-157019 US 2002-199481

OTHER SOURCE(S):

MARPAT 132:322147

Amino acid hydroxyethylamino sulfonamide compds. I [R2 = (un)substituted aryl, (cyclo)alkyl, aralkyl, cycloalkylalkyl; R3 = alkyl, haloalkyl, alkenyl, alkynyl, hydroxy-, alkoxy-, alkythio-, or alkylaulfonylalkyl, cycloalkylalkyl, heterocycloalkylalkyl, eterocycloalkylalkyl, aryl, aralkyl, or heterocycloalkyl, heterocycloalkyl, heterocycloalkyl, heterocycloalkyl, heterocycloalkyl, aryl, aralkyl, or heterocycloalkyl, heteroc

19905-92-28
RI: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(amino acid hydroxyethylamino sulfonamides as retroviral protease inhibitors)

inhibitors) 159005-92-2 CAPLUS

Carbanic acid, [(15)-3-amino-1-[[((15,2R)-2-hydroxy-3-[(3-math)]buty]) [phenylsulfony]) amino]-1-[phenylsulfony]) amino]-1-[phenylsulfony]] amino] carbony]]-3-oxopropy]]-, phenylmathy] ester (SCI) (CA INDEX MAME)

Absolute stereochemistry.

L7 ANSWER 3 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN ACCESSION NUMBER: 2000:304314 CAPLUS DOCUMENT NUMBER: 132:322147 Preparation of  $\alpha$ - and  $\beta$ -amino acid hydroxyethylamino sulfonamides as retro viral protease inhibitors. DOCUMENT NUMBER: TITLE: inhibitors.
Vazquez, Michael L.; Mueller, Richard A.; Talley, John J.; Getman, Daniel P.; Decrescenzo, Gary A.; Freskos, John N.; Heintz, Robert M.; Bertenshaw, Deborah E. G.D.Searle and Co., USA
U.S., 93 pp., Cont.-in-part of Appl. PCT/US93/07814.
CODER: USXMAM INVENTOR (S): PATENT ASSIGNEE(S): DOCUMENT TYPE:

FAMILY ACC. NUM. COUNT: PATENT INFORMATION: US 6060476 A 20000509 US 1994-204827 19940302
WO 9404492 A1 19940303 WO 1993-US7814 19930824
W: AT, AU, BB, BG, BR, BY, CA, CH, CZ, DE, DK, ES, FI, GB, HU, JP,
XP, KR, KZ, LK, LU, HG, NN, MW, NL, NO, NZ, PL, PT, RO, RU, SD,
SE, SK, LAU, US, VN
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE,
BP, BJ, CF, CG, CI, CM, GA, M, HL, MR, NR, SN, TD, TG
EP 810209 A2 19971203 KP 1997-113434 19930824
EP 810209 B1 20020605
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE
WO 9506030 A1 19950302 WO 1994-US9139 19940823
V: AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, ES, FI, GB,
GE, HU, JP, KE, KG, KP, KR, KZ, LK, LT, LI, LU, LV, MD, MG, MM, MW,
NL, NO, NZ, PL, PT, RO, RU, SD, SE, SI, SK, TJ, TT, UA, US, US,
UZ, VN
RW: KE, MW, SD, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC,
NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, M, ML, MR, NE, SN, TD, TG
AU 9476697 A1 19960612 EP 1934-027162 19940823
EP 715618 B1 19991216
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE
AT 174587 E 19990115 AT 1994-927162 19940823
US 96455801 B1 20020802 AT 174587 ES 2127938 US 5968942 US 6455581 US 6248775 US 6500832 US 2002052399 US 6417387 A1 B2 A1 B2 A1 B2 B1 A1 US 2003191319 US 6646010 US 6646010 US 2004044047 US 6846954 US 6924286 US 2003-633376 US 2004-812343 US 1992-934984 WO 1993-US7814 EP 1993-923714 US 1993-110911 US 1994-204827 US 1994-294468 20030804 20040330 20050802 20041118 US 2004229922 PRIORITY APPLN. INFO.: B2 19920825 A2 19930824 A3 19930824 A 19930824

ANSWER 3 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

159005-89-7P 159005-91-1P 159005-95-3P
159006-21-0P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SFN (Synthetic preparation); TRU (Therapeutic use);
BIOL (Biological study); PREP (Preparation); USES (Uses)
(amino acid hydrowysthylamino sulfonamides as retroviral protease inhibitors)
159005-89-7 CAPLUS
Butanediamide, NI-([IS, 2R)-2-hydroxy-3-[(3-methylbutyl)(methylsulfonyl)amino]-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI)
(CA INDEX NAME)

159005-91-1 CAPLUS Butanediamide, N1-[(1S,2R)-2-hydroxy-3-[(3-methylbutyl) (phenylsulfonyl)amino]-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

ANSWER 3 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

159005-95-5 CAPLUS Butanediamide, NI-[(15,2R)-2-hydroxy-3-[(3-methylbutyl)(phenylsulfonyl)amino]-1-(phenylmethyl)propyl]-N4-methyl-2-[(2-quinolinylcarbonyl)amino]-, (25)-(9CI) (CA INDEX NAME)

### Absolute stereochemistry.

159006-21-0 CAPLUS
Carbamic acid, [(15)-3-amino-1-[[[(15,2R)-2-hydroxy-1-(phenylmethyl)-3-(phenylsulfonyl)propylamino]propyl]amino]carbonyl]-3-oxopropyl]-, phenylmethyl ester [9CI) (CA INDEX NAME)

#### Absolute stereochemistry.

159005-90-09 159006-05-09 159006-22-19
RL: RCT (Reactant): SPN (Synthetic preparation): PREP (Preparation): RACT (Reactant or reagent)
(amino acid hydroxyethylamino sulfonamides as retroviral protease

ANSWER 3 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

REFERENCE COUNT:

THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 3 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN

Inhibitors CAPUMS CERTIFICATION AND SHEET THE STATE OF TH

(Continued)

#### Absolute stereochemistry.

159006-05-0 CAPLUS Butanediamide, 2-amino-N1-[{15,2R}-2-hydroxy-3-[(3-methylbutyl) (methylsulfonyl) amino}-1-(phenylmethyl)propyl]-, (25)- (9CI) (CA INDEX NAME)

#### Absolute stereochemistry.

159006-22-1 CAPLUS
Carbamic acid, [(15)-1-[[[(15,2R)-2-hydroxy-3-{[3-methylbutyl] (phemylsulfonyl) amino]-1-(phenylmethyl) propyl] amino] carbonyl]-3-(methylamino)-3-oxopropyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX

## Absolute stereochemistry.

DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

	ENT :						DATE									ATE	
		+				-									-		
υs	6046	190			Α		2000	0404		US 1	996-	5868	66		1	9960	124
WO	9404	492			A1		1994	0303	,	WO 1	993-	US78	14		1	9930	824
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		KP,	KR,	KZ,	LK,	LU,	MG,	MN,	MW,	NL,	NO,	NZ,	PL,	PT.	RO,	RU,	SD,
		SE,	SK,	UA,	US,	VN											
	RW:	AT,	BE,	CH,	DE,	OK,	ES,	FR,	GB,	GR,	IE,	IT,	LU,	MC,	NL,	PT,	SE,
		BF,	BJ,	CF,	ÇG,	CI,	CM,	GA,	GN,	ML,	MR,	NE,	SN,	TD,	TG		
EΡ	8102	09			A2		1997	1203		EP 1	997-	1134	34		1	9930	824
EP	8102	09			A3		1998	1202									
EP	8102	09			B1		2002	0605									
	R:	AT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	IT,	LI,	LU,	NL,	SE,	PT,	IE
WO	9506	030			A1		1995	0302		WO 1	994-	US91	39		1	9940	823
	₩:	AM,	AT,	AU,	BB,	BG,	BR,	BY,	CA,	CH,	CN,	CZ,	DE,	DX,	ES,	FI,	GB,
		GE,	ΗU,	JP,	ΚE,	KG,	KP,	KR,	ΚZ,	LK,	LT,	LU,	LV,	MD,	MG,	MN,	MW,
		NL,	NO,	NZ,	PL,	PT,	RO,	RU,	50,	SE,	SI,	SK,	TJ,	TT,	UA,	US,	US,

AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, BF, BJ, CF, CG, CI, CH, GA, GN, ML, MR, NE, SN, TD, TG

US 1992-934984 B2 19920925

WO 1993-U57814 A2 19930824

US 1994-204872 B2 19940302

WO 1994-U59139 V 19940823

EP 1993-923714 A3 19930824

US 1993-110911 A 19930824

US 1993-101911 A 19930824

HARPAT 132:265504

OTHER SOURCE(S): MARPAT 132:265504

AB Hydroxyethylamino sulfonemide compds. R9RION(CR7R8)pCHRIC(:Y)NR6CHR2CH(OH)
CH2NR35(:O)RR4 [I: RI = H, CH2SOZNH2, CH2COZCH3, alkyl, haloalkyl,
alkenyl, alkynyl, cycloalkyl, amino acid side chains, etc.; R2 =
(un)substituted alkyl, aryl, cycloalkyl, cycloalkyl, cycloalkyl, aralkyl, aralkyl, R3 = H,
alkyl, haloalkyl, alkenyl, alkynyl, aryl, heteroaryl, mono- and
disubstituted aminoalkyl, etc.; R4 = alkyl, haloalkyl, alkenyl, alkynyl,
aryl, (un)saturated heterocycle, (un)substituted aromatic heterocycloalkyl,
etc.;

, R6 - H, alkyl; Y - O, S, NR3; R7,R8 = independently H, R1, or together with R1 and the carbon atoms to which they are attached represent a cycloalkyl radical; R9 = H, R3, or R3SO2; R10 = H, alkowycarbonyl, atolak alkylcarbonyl, arotol, aryloxycarbonyl, heterocyclylalkowycarbonyl, monoand disubstituted aminocarbonyl, or aminoalkanoyl, etc.; or R9R10N = heterocycloalkyl or heteroaryl; x = 0-2; p = 0-1] or their pharmaceutically acceptable saits, prodrugs, or esters were prepared as inhibitors of retroviral proteases such as human immunodeficiency virus

- ANSWER 4 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

  (HIV). Hany inhibitors were prepd. by (1) prepg. an N-protected amino epoxide and (2) reacting this with an amine and (3) prepg. a sulfonamide by reacting with a sulfonyl chloride or sulfonyl andyride in the presence of an acid scavenger. The amino function of the sulfonamide was then (4) deprotected and (5) reacted with a carbonylate. Thus, (13-mthylbutyl) (phenylsulfonyl) amino) 15
  (phenylmethyl)propyl)-25-(2-quinolinylcarbonyl) amino) 15
  prepd. and assayed for HIV protease inhibitory activity (IC50 = 1.5 nM). Compds. of formula I were tested for cytotoxicity and antiviral efficacy (IC50, ESO, and TD50 values at the nanocolar level are tabulated). 159005-89-7P 159005-91-1P 159005-92-2P

  RI: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); TBU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

  (preparation of hydroxyethylamino sulfonamides useful as retroviral

(preparation of hydroxyethylamino Solimino Solim

## Absolute stereochemistry.

159005-91-1 CAPLUS
Butanediamide, N1-[(15,2R)-2-hydroxy-3-[(3-methylbutyl)(phenylsulfonyl)amino]-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (25)- (9CI)(CA INDEX NAME)

159005-92-2 CAPLUS Carbamic acid, [(15)-3-amino-1-[[[(15,2R)-2-hydroxy-3-[(3-

## ANSWER 4 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN

IT 159005-90-0P 159006-05-0P 159006-06-1P
RL: RCT (Reactant): SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
protease inhibitors)
RN 159005-90-0 CAPLUS
CN 2-Thia-3,7,10-triazaundecan-11-oic acid, 9-(2-amino-2-oxoethyl)-5-hydroxy-3-(3-methylbutyl)-8-oxo-6-(phenylmethyl)-, phenylmethyl ester, 2,2-dioxide, (5R,6S,9S)- (9CI) (CA INDEX NAME)

## Absolute stereochemistry.

159006-05-0 CAPLUS Butanediamide, 2-amino-N1-[(15,2R)-2-hydroxy-3-[(3-methylbutyl) (methylbulfonyl) amino]-1-(phenylmethyl)propyl]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSVER 4 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
methylbutyl) (phenylsulfonyl) amino] -1-(phenylmethyl) propyl] =mino] carbonyl] 3-oxopropyl] -, phenylmethyl ester (9CI) (CA INDEX NAME)

## Absolute stereochemistry.

159005-95-5 CAPLUS Butanediamide, N1-([15,2R]-2-hydroxy-3-[{3-methylbutyl} (phenylsulfonyl) amino]-1-(phenylmethyl) propyl]-N4-methyl-2-[{2-quinolinylcarbonyl) amino]-, (25)-(9CI) (CA INDEX NAME)

## Absolute stereochemistry.

159006-21-0 CAPLUS
Carbanic acid, [(15)-3-amino-1-[[[(15,2R)-2-hydroxy-1-(phenylmethyl)-3-[(phenylmifonyl)propylamino|propyl]amino|carbonyl]-3-oxopropyl]-,
phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

## ANSWER 4 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN · (Continued)

159006-06-1 CAPLUS
Butanediamide, 2-amino-N1-[(1S,2R)-2-hydroxy-3-[(3-methylbutyl) (phenylsulfonyl) amino]-1-(phenylsulfonyl) propyl]-, (2S)- (9CI) (CA INDEX NAME)

## Absolute stereochemistry.

REFERENCE COUNT:

THERE ARE 45 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 5 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN SSION NUMBER: 1999:811207 CAPLUS MENT NUMBER: 132:49801

English

DOCUMENT NUMBER: TITLE:

132.49801
Preparation of 1-acylamino-3-(N-arylsulfonyl-N-alkoxymino)-2-hydroxypropanes and related compounds as inhibitors of HIV aspartyl protease.
Sherrill, Ronald Georger Hale, Michael R.;
Spaltenstein, Andrews Furfine, Eric Steven; Andrews, Clarence Webster, III; Lowen, Gregory Thomas
Vertex Pharmaceuticals Incorporated, USA
CODEN: PIXXO2
Patent INVENTOR (S):

PATENT ASSIGNEE(S):

DOCUMENT TYPE: LANGUAGE:

FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

	PA:	TENT	NO.			KIN	D	DATE				ICAT						
							-											
	WO	9965	870			A2		1999	1223		WO 1	1999-	US13	744			19990	617
	WO	9965																
		W:	λĔ,	AL,	AH,	AT,	AU,	ΑZ,	BA,	BB,	BG.	BR,	BY,	CA,	CH,	CN.	. cu.	CZ.
			DE,	DK,	EE,	ES,	FI,	GB,	GD,	GE,	GH,	GM,	HR,	HU.	ID.	IL.	IN.	15.
			JP,	KE,	KG,	KP,	KR,	KZ.	LC.	LK.	LR,	L5,	LT.	LU.	LV.	MD.	MG.	MK.
			MN,	MW.	MX,	NO,	NZ,	PL.	PT.	RO,	RU,	SD,	SE,	SG.	SI.	SK.	SL.	TJ.
			TM,	TR,	TT,	UA,	UG,	US.	UZ,	VN.	YU,	ZA,	ZW.	AM.	AZ.	BY.	RG.	KZ.
				RU.					-		-							
		RW:	GH.	GM.	KE.	LS.	MW.	SD.	SL.	sz.	UG.	ZW,	AT.	BE.	CH.	CY.	DR.	ĐK.
			ES.	FI.	FR.	GB.	GR.	IE.	IT.	w.	HC.	NL,	PT.	SE.	BF.	BJ.	CF.	CG.
			CI.	CH.	GA.	GN.	GW.	ML.	MR.	NE.	SN.	TD.	TG					
	CA	2335	477			λA		1999	1223		CA I	999-	2335	477		1	19990	617
	AU	9945	760			A1		2000	0105		AU I	999-	4576	0		- 1	19990	617
	AU	7677	28			B2		2003	1120					-				
	EP	1086	076			A1		2001	0328		EP 1	999-	9287	69		1	19990	617
	EP	1086	076			B1		2004	1222									
	-										GR.	IT,	T.T.	TAT .	NI	SR	MC.	PT.
			7.77	17.4											-		-	-
	BR	9912	169			A		2001	0410		BR 1	999-	1216	9		1	9990	617
	NZ	5088	55			Ä		2003	1031		NZ 1	999-	5088	55		- 1	9990	617
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	US	2002	0492	01		A1		2002	0425		us 2	-000	7311	29		- 3	20001	206
	115	6617	1743			R2		2003	ハタハフ									
	NO	2000	0064	05		A		2001	0219		NO 2	-000	6405				20001	215
	US	2004	0975	94		A1		2004	0520		US 2	000- 003- 003-	6009	37		- 3	20030	620
	NZ	5280	74			A		2004	1126		N2 2	2003-	5280	74		- 3	20030	908
RIC	RIT	Y APP	I.N.	INFO							115 1	998-	9009	AP		p 1	OBBO	619
											WO I	999-	US13	744		ù i	9990	617
											us 2	999-	7311	29		A3 2	20001	206

US 2000-731129 A3 20001206

OTHER SOURCE(S): MARPAT 132:49801

ABMN(GM)CHDCHOR7CH2ND'SOZE {A = H, (substituted) Ht, R1Ht, R1Ak; Ak = alkyl; Ht = cycloalkyl, cycloalkenyl, (substituted) aryl, heterocyclyl; R1 = CO, SOZ, COCO, OZC, NRZCOZ, etc.; B = null, NRZC(R3)2CO; x = 0, 1; R2 = H, (substituted) Ht, alkyl; R3 = H, (substituted) Ht, alkyl, alkenyl, cycloalkeyl; G = null, H, R7, alkyl; G may be bound to R7; D = (substituted) Q, alkyl, alkenyl; Q = (substituted) carbocyclyl, heterocyclyl; D' = ORIO, NRIO, NRIO, NRIO, NRIO, R1R3; E = Ht, ORIC, ORIO, NRZCAZ, (substituted) alkyl, alkenyl, etc.; R7 = H, (CH2O)xY(ZM)(IX)Z(M)x, etc.; M = null, H, Li, Na, K, My, Ca, Ba, alkyl, alkenyl, etc.; X = O, S; Y = P, S; Z = O, S, NR22, H, were prepared as inhibitors of HTV aspartyl protease (no data). Thus, 3-H2NCGH4SOZNHOCHMe2 (preparation given), tert-Bu

ANSWER 5 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN

(Continued) PAGE 1-A

PAGE 1-B

252871-35-5 CAPLUS
Butanediamide, N1-[(15,2R)-3-[(cyclopentyloxy)(1H-indazol-6-ylsulfonyl]amino]-2-hydroxy-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

252871-52-6 CAPLUS
Butanediamide, N1-[(15,2R)-3-[(cyclohemyloxy)[(4-methoxyphenyl)sulfonyllamino]-2-hydroxy-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (25)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSVER 5 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
N-[15]-1-[(25]-owiran-2-yl]-2-phenylethylcarbanate, and phosphazene base
P4 tert-Bu were stirred in 8 h in THF to give 95t tert-Bu
N-[15,2R)-3-[[(3-aminophenyl]sulfonyl](isopropoxy) amino]-1-benzyl-2hydroxypropylcarbanate.
252871-32-2P 252871-33-3P 252871-34-4P
252871-35-5P 252871-55-6P 252871-57-IP
252871-35-1P 252871-53-9P

252871-63-9p
RL: BAC (Biological activity or effector, except adverse); BSU (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SFN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation) of ISSS (Uses) (preparation of 1-acylamino-3-(N-arylaulfonyl-N-alkoxyamino)-2-hydroxypropanes and related compds. as inhibitors of HIV aspartyl protease)
252871-32-2 CAPUS
Butanediamide, N1-[(1S.2R)-3-[((3-aminophenyl)sulfonyl)(cyclopentyloxy)amino]-2-hydroxy-1-(phenylmethyl)propyl)-2-[(2-quinolinylcarbonyl)amino)-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

252871-33-3 CAPLUS
Butanediamide, NI-([15,2R)-3-[(cyclopentyloxy)[[4-methoxyphenyl]sulfonyl]anino]-2-hydroxy-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

252871-34-4 CAPLUS
Carbantc acid, [5-[[[(2R,3S)-3-[[(2S)-4-amino-1,4-dioxo-2-[(2-quinoilnylcarbonyl) aminojbutyl] aminoj-2-hydroxy-4-phenylbutyl](cyclopentyloxy) aminoj bulfonyl]-IH-benzimidazol-2-yl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 5 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

252871-57-1 CAPLUS Butanediamide, N1-([15,2R)-2-hydroxy-3-[[(4-methoxyphenyl)sulfonyl](1-meth)plropxy)amino]-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

252071-63-9 CAPLUS
Butanediamide, N1-[(15,2R)-2-hydroxy-3-[[(4-methoxyphenyl)sulfonyl]{(tetra hydro-ZH-pycan-4-yl)oxy]amino]-1-(phenylmethyl)propyl)-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME) -

L7 ANSWER 6 OF 19 CAPLUS COPYRIGHT 2005 ACS ON STN ACCESSION NUMBER: 1999:722916 CAPLUS DOCUMENT NUMBER: 131:336822
TITLE: Preparation

Preparation of succinamide inhibitors of INVENTOR (5):

Preparation of succinamide inhibitors of interleukin-1B converting enzyme
Caprathe, Bradley Williams Gilmore, John Lodge;
Earter, William Glen; Hays, Sheryl Jeanne; Knapp,
Kristen Hichele; Kostlan, Catherine Rose; Lunney,
Elizabeth Ann; Para, Kimberly Suzanne; Galatis, Paul;
Thomas, Anthony Jerome
Warner-Lambert Company, USA; BASF Aktiengesellschaft
PCT Int. Appl., 116 pp.
CODEN: PIXXO2

PATENT ASSIGNEE(S): SOURCE:

DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION: Patent English

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			NO,	NZ,	PL,	RO.	SG,	SI.	SK,	SL,	TR	, TT.	UA.	us.	UZ.	VN.	YU.	ZA,
								MD,										
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	EΡ	1082	127			B1		2005	0622									
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			IE,	SI,	LT,	LV,	FI,	RO										
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	JΡ	2002	5137	66		T2		2002	0514		JΡ	2000-	5467	89		1	9990	430
	AΤ	2982	42			E		2002	0715		λT	1999-	9189	30		1	9990	430
	NO	2000	0055	37		A		2000	1220		NO	2000- 2000-	5537			2	0001	102
	HR	2000	0007	44		A1		2001	0630		HR	2000-	744			2	0001	103
	ZΑ	2000	0068	91		A		2002	0525		ZA.	2000-	6881			2	0001	123
	BG	1050	02			λ		2001	0731		BG	2000-	1050	02		2	0001	
PRIOR	ITY	APP	LN.	INFO	. :						US	1998-	8432	OP		P 1	9980	505
											WO	1999-	US94	63	1	w 1	9990	430
OTHER GI	SC	URCE	(5):			MARI	PAT	131:	3368									

ANSWER 6 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
Pentanoic acid, 3-[[(25)-4-amino-2-(1-methylethyl)-1,4-dioxobutyl]amino]-5[[[(15,8,4)-7,7-dimethyl-2-oxobicyclo[2,2.1]hept-1yl]methyl]sulfonyl]amino]-4-oxo- (9CI) (CA INDEX NAME)

249539-58-0 CAPLUS Pentanoic acid, 5-[[[(15,4R)-7,7-dimethyl-2-oxobicyclo{2.2.1}hept-1-yl]methyl]sulfonyl]amino]-3-[[(25)-2-(1-methylethyl)-1,4-dioxo-4-[(2-phenylethyl)amino]butyl]amino]-4-oxo- (9CI) (CA INDEX NAME)

## Absolute stereochemistry.

249539-59-1 CAPLUS

Pentanoic acid, 3-[((2s)-4-amino-2-(1-methylethyl)-1,4-dioxobutyl]amino]-4-oxo-5-[((2-phenylethyl)sulfonyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L7 ANSWER 6 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

The title compds. [I; Y = II-IV (wherein Rl1 = H. alkyl; X = H. (CH2)nM(Rl1)SO2(CH2)n-aryl, (CH2)nM(Rl1)SO2(CH2)n-substituted aryl, etc.); Rl, R2 = H. alkyl; (CH2)n-substituted aryl, etc.; n = 0-6; R3 = H. alkyl; R4 = alkyl; H] and their salts, useful for treating stroke, inflammatory diseases such as rheumatoid arthritis or inflammatory bowel disease, septic shock, reperfusion injury, Altehiemer's disease, shigellosis, and multiple sclerosis, were prepared E.g., a detailed 6-step synthesis of I [R1 = Ph(CH2)2; R2 = R3 = H; R4 = He; Rl1 = H; Y = CH(CH2)2DERISO2(CH2)2Ph) which showed ICSO of 14.50 µM against ICE, was given.

[R1 = Ph(CH2)2; R2 = R3 = H; R4 = He; R11 = H; Y = CH(CH2002H)COCCIPANSO2 (CH2)2Ph) which showed IC50 of 14.50 µM against IC5, was given.

1C5, was given.

249539-55-77 249539-66-87 249539-58-07

249539-55-77 249539-66-07 249539-67-17

249539-73-97 249539-74-07 249539-75-17

249539-73-97 249539-74-07 249539-75-17

249539-73-17-17 249539-88-67 249539-75-17

249539-71-17 249539-98-97 249539-95-57

249539-91-17 249539-93-37 249540-06-57

249540-09-87 249540-05-47 249540-06-57

249540-09-87 249540-05-47 249540-06-57

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, by REF (Preparation); THU (Therapeutic use); BIOL (Biological study); PREF (Preparation); USES (Uses)

[preparation of succinamide inhibitors of interleukin-16 converting enzyme)

249539-55-7 CAPLUS

Pentanoic acid, 3-[(2-methyl-1,4-dioxo-4-[(2-phenylethyl)amino]butyl]amino]

]-4-oxo-5-[[(2-phenylethyl)sulfonyl]amino] - (9CI) (CA INDEX NAME)

249539-56-8 CAPLUS

ANSWER 6 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

249539-60-4 CAPLUS
Pentanoic acid, 3-[[(2S)-2-(1-methylethyl)-1,4-dioxo-4-[(2-phenylethyl) amino]-butyl]amino]-4-oxo-5-[[(2-phenylethyl) sulfonyl]amino]-(9CI) (CA INDEX NAME)

249539-61-5 CAPLUS
Pentanoic acid, 5-[[[7,7-dimethylbicyclo[2,2.1]hept-1yl]methyl]sulfonyl]amino]-3-[[(25)-2-(1-methylethyl)-1,4-dioxo-4-[[2phenylethyl]amino]butyl]amino]-4-oxo- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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249539-64-8 CAPLUS Pentanoic acid, 5-[[[[15,4R]-7,7-dimethyl-2-oxobicyclo[2.2.1]hept-1-yl]methyl]ulfonyl]amino]-3-[[[25]-2-(1-methylethyl)-1,4-dioxo-4-[(2-phenoxyethyl)amino]butyl]amino]-4-oxo- (9CI) (CA INDEX NAME)

249539-66-0 CAPLUS
Pentanoic acid, 5-[[[(15,4R)-7,7-dimethyl-2-oxobicyclo[2.2.1]hept-1-yl]methyl]uslfonyl]amino]-3-[(25)-2-[1-methylethyl)-4-[methyl(2-phenylethyl) amino]-1,4-dioxobutyl]amino]-4-oxo- (9CI) (CA INDEX NAME)

#### Absolute stereochemistry.

249539-67-1 CAPLUS Pentanoic acid, 5-[[[(15,4R)-7,7-dimethyl-2-oxobicyclo[2.2.1]hept-1-yl]methyl]sulfonyl]amino]-3-[[(25)-2-(1-methylethyl)-1,4-dioπο-4-[(3-phenylpropyl)amino]butyl]amino]-4-oxo-(9CI) (CA INDEX NAME)

## Absolute stereochemistry.

ANSWER 6 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
Pentanoic acid. 5-[[[[15,48]-7.7-dimethy]-2-oxobicyclo[2.2.1]hept-1yl]nethyl]aulfonyl]amino]-3-[[(25)-4-[[3-(4-hydroxyphenyl)propyl]amino]-2[1-methylethyl]-1,4-dioxobutyl]amino]-4-oxo-(9CI) (CA INDEX NAME)

# Absolute stereochemistry.

249539-76-2 CAPLUS
Pentanoic acid, 5-[[[[(1s,4R)-7.7-dimethyl-2-oxobicyclo[2.2.1]hept-1-yl]methyl]ulfonyl]amino]-3-[[(2S)-2-(1-methylethyl)-4-[[2-(2-naphthalenyl)ethyl]amino]-1,4-dioxobutyl]amino]-4-oxo- (9CI) (CA INDEX NAME)

## Absolute stereochemistry.

# PAGE 1-B

249539-77-3 CAPLUS Pentanoic acid, 5-[[[(15,4R)-7,7-dimethyl-2-oxobicyclo[2.2.1]hept-1-yl]methyl]ulfonyl]amino]-3-[[(25)-2-(1-methyl-thyl)-4-[[2-(7-methyl-1H-indol-3-yl)ethyl]amino]-1,4-dioxobutyl]amino]-4-oxo-(9CI) (CA INDEX NAME)

17 ANSWER 6 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

249539-73-9 CAPLUS
Pentanoic acid, 5-[[[(15,4R)-7,7-dimethyl-2-oxobicyclo[2.2.1]hept-1yl]methyl]sulfonyl]amino]-3-[(25)-4-(hydroxyamino)-2-(1-methylethyl)-1,4dioxobutyl]amino]-4-oxo-(9CI) (CA INDEX NAME)

## Absolute stereochemistry.

249539-74-0 CAPLUS Pentanoic acid, 5-[[[[15,4R]-7,7-dimethyl-2-oxobicyclo[2.2.1]hept-1-yi]methyl]uslfonyl]amino]-3-[[(2S)-4-[[2-(1H-indol-3-yl)ethyl]amino]-2-(1-methylethyl)-1,4-dioxobutyl]amino]-4-oxo-(9CI) (CA INDEX NAME)

249539-75-1 CAPLUS

ANSWER 6 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

249539-79-5 CAPLUS
Pentanoic acid, 5-[[[(15,48)-7,7-dimethyl-2-oxobicyclo(2.2.1]hept-1-yl]methyl]aulfonyl]amino]-3-[([25)-4-[(2-(6-fluoro-1H-indol-3-yl)ethyl]amino]-2-(1-methylethyl)-1,4-dioxobutyl]amino]-4-oxo-(9CI) (CA

PAGE 1-B

249539-85-3 CAPLUS
Pentanoic acid, 5-[[[7,7-dimethylbicyclo[2.2.1]hept-1yl]methyl]sulfonyl]amino]-3-[[(25)-2-(1-methylethyl)-1,4-dioxo-4-[(3-phenylpropyl)amino]butyl]amino]-4-oxo-(9CI) (CA INDEX NAME)

249539-88-6 CAPLUS
Pentanoic acid, 5-[[(7,7-dimethylbicyclo[2.2.1]hept-1yl]methyl]sulfonyl]amino]-3-[[(25)-2-(1-methylethyl)-4-[(2-(1-methyl-1Hindol-3-yl)ethyl]amino]-1,4-dioxobutyl]amino]-4-oxo- (9CI) (CA INDEX

#### Absolute stereochemistry.

249539-90-0 CAPLUS Pentanoic acid, 5-[[[(15,4R)-7,7-dimethyl-2-oxobicyclo[2.2.1]hept-1-y]lmethyl]sulfonyl]amino]-3-[[(25)-2-(1-methylethyl)-1,4-dioxo-4-[(3-(4-pyridinyl)propyl]amino]butyl]amino]-4-oxo- (9CI) (CA INDEX NAME)

#### Absolute stereochemistry.

249539-91-1 CAPLUS Pentanoic acid, 5-[[[[(15,4R)-7,7-dimethyl-2-oxobicyclo[2.2.1]hept-1-

#### ANSWER 6 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

249539-97-7 CAPLUS
Pentanoic acid, 5-[[[[15,4R]-7,7-dimethyl-2-oxobicyclo[2.2.1]hept-1-yl]methyl]ulfonyl]amino]-3-[[(25)-2-(1-methylathyl)-1,4-dioxo-4-[[3-(3-pyridinyl)propyl]amino]butyl]amino]-4-oxo- (9CI) (CA INDEX NAME)

249539-98-8 CAPLUS
Pentanoic acid, 5-{[[((15,4R)-7,7-dimethyl-2-oxobicyclo{2.2.1}hept-1-yl]methyl]sulfonyl]amino]-3-[((25)\*2-(1-methylethyl)-1,4-dioxo-4-[(3-(3-yptidinyl)propyl)amino]butyl]amino]-4-oxo-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CRN 249539-97-7 CMF C30 H44 N4 O8 S

## Absolute stereochemistry.

ANSVER 6 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN (Continued) yl]methyl]sulfonyl]amino]-3-[{(25)-2-(1-methylethyl)-1,4-dioxo-4-[(3-(4-pyridinyl)propyl]amino]butyl]amino]-4-oxo-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

Q4 1

CRN 249539-90-0 CMF C30 H44 N4 08 5

#### Absolute stereochemistry.

CH. 2

CRN 76-05-1 CMF C2 H F3 02

249539-93-3 CAPLUS
Pentanoic acid, 5-[[[(15,4R)-7,7-dimethyl-2-oxobicyclo[2.2.1]hept-1-yl]methyl]sulfonyl]amino]-3-[[(25)-2-(1-methylethyl)-1,4-dioxo-4-[(3-(2-quinolinyl)propyl]amino]butyl]amino]-4-oxo- (9CI) (CA INDEX NAME)

249539-95-5 CAPLUS
Pentanoic acid. 5-[[[(15,4R)-7,7-dimethyl-2-oxobicyclo[2.2.1]hept-1-yl]methyl]sulfonyl]amino]-3-[[(25)-2-(1-methylethyl)-4-[(3-(2-naphthalenyl))propyl]amino]-1,4-dioxobutyl]amino]-4-oxo- (9CI) (CA INDEX NAME)

ANSWER 6 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN CM 2 (Continued)

249540-01-0 CAPLUS
Pentanoic acid, 3-[[(2S)-4-[[2-(1H-benzimidazol-1-yl)ethyl]amino]-2-(1-methylethyl)-1, 4-dioxobutyl]amino]-5-[[[([1S,4R)-7,7-dimethyl-2-oxobicyclo[2.2.1]hept-1-yl]methyl]buffonyl]amino]-4-oxo-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CRN 249540-00-9 CMF C31 H43 N5 O8 S

CH 2

CRN 76-05-1 CMF C2 H F3 02

249540-03-2 CAPLUS
Pentanoic acid, 5-{[[([15,4R)-7,7-dimethyl-2-oxobicyclo(2.2.1]hept-1-yl]methyl]sulfonyl]amino]-3-{[(25)-2-(1-methyl-thyl)-4-{[2-(1-methyl-1H-indol-3-yl)ethyl]amino]-1,4-dioxobutyl]amino]-4-oxo-(9CI) (CA INDEX NAME)

249540-05-4 CAPLUS
Pentanoic acid, 5-[[[(15,4R)-7,7-dimethyl-2-oxobicyclo[2.2.1]hept-1yl]methyl]sulfonyl]amino]-3-[{(25)-2-(1-methylethyl)-1,4-dioxo-4-[[2-(4pyridinyl)ethyl]amino]butyl]amino]-4-oxo-(9CI) (CA INDEX NAME)

#### Absolute stereochemistry.

249540-06-5 CAPLUS
Pentanoic acid, 5-[[[[15,4R]-7,7-dimethyl-2-oxobicyclo[2.2.1]hept-1yl]methyl]sulfonyl]mmino]-3-[[(25)-2-(1-methylethyl)-1,4-dioxo-4-[[2-(4pycidinyl)ethyl]mino]butyl]amino]-4-oxo-, trifluoroacetate (2:3) (9CI)
(CA INDEX NAME)

СН

CRN 249540-05-4 CMF C29 H42 N4 O8 S

Absolute stereochemistry.

ANSWER 6 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN

(Continued)

(Continued)

PAGE 1-B

=0

249540-12-3 CAPLUS
Pentanoic acid, 5-[[[(15,4%)-7,7-dimethyl-2-oxobicyclo[2.2.1]hept-1yl]methyl]aulfonyl]amino]-3-[[(25)-2-(1-methylethyl]-1,4-dioxo-4-[[2-(1Htetrazol-5-yl)ethyl]amino]butyl]amino]-4-oxo-, mono(trifluoroacetate)
(9CI) (CA INDEX NAME)

CM 1

CRN 249540-11-2 CMF C25 H39 N7 O8 S

Absolute stereochemistry.

CH 2

CRN 76-05-1 CMF C2 H F3 O2

249540-55-4 CAPLUS
Pentanoic acid, 5-[[[(15,4R)-7,7-dimethyl-2-oxobicyclo[2.2.1]hept-1yl]methyl]ulfonyl]amino]-3-[[2-(1-methylethyl)-4-[methyl[2-(1-methyl-1Hindol-3-yl)ethyl]amino]-1,4-dioxobutyl]amino]-4-oxo-(9CI) (CA INDEX
RMHE)

ANSWER 6 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN

(Continued)

CH 2

CRN 76-05-1 CMF C2 H F3 O2

249540-09-8 CAPLUS Pentanoic acid, 3-[[(2S)-4-[[2-(5-acetyl-1H-indol-3-yl)ethyl]amino]-2-(1-methylethyl)-1, 4-dioxobutyl]amino]-5-[[[[(1S,4R)-7,7-dimethyl-2-oxobicyclo[2.2.1]hept-1-yl]methyl]sulfonyl]amino]-4-oxo-(9CI) (CA INDEX NAME)

PAGE 1-A 

ANSWER 6 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

249540-56-5 CAPLUS
Pentanoic acid, 5-[[[[(15,48)-7,7-dimethyl-2-oxobicyclo[2.2.1]hept-1-y]methyl]uslfonyl]amino]-3-[[2-ethyl-1,4-dioxo-4-[(3-phenylpropyl)amino]butyl]amino]-4-oxo-(9CI) (CA INDEX NAME)

249540-57-6 CAPLUS
Pentanoic acid, 5-[[[([15,4R)-7,7-dimethyl-2-oxobicyclo[2.2.1]hept-1-yl]methyl]aufonyl]amino]-3-[[2-ethyl-4-[[2-(1-methyl-lH-indol-3-yl)ethyl]amino]-1,4-dioxobutyl]amino]-4-oxo- (9CI) (CA INDEX NAME)

249540-64-5P 249540-69-0P 249540-81-6P 249540-84-9P 249540-85-0P

249540-84-99 249540-83-09 RB: RCT (Reactant): SPN (Synthetic preparation): PREP (Preparation): RACT (Reactant or reagent) (preparation of succinamide inhibitors of interleukin-18 converting enzyme)
249540-64-5 CAPLUS

249540-69-0 CAPLUS
2-Oxa-3,8,12-triazatridecan-13-oic acid, 12-[[[(15,4R)-7,7-dimethyl-2-oxobicyclo[2.2.1]hept-1-yl]methyl]-ulfonyl]-6-(1-methylethyl)-4,7,10-trioxo-9-[2-oxo-2-(henylmethoxy)ethyl]-1-phenyl-, 1,1-dimethylethyl ester, (65)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

249540-81-6 CAPLUS
Pentanoic acid, 5-[[(1,1-dimethylethoxy) carbonyl][[[(15,4R)-7,7-dimethyl-2-oxobicyclo[2.2.1]hept-1-yl]methyl]sulfonyl]amino]-3-[[(25)-2-(1-methylethyl)-1,4-dioxo-4-[(2-phenoxyethyl)amino]butyl]amino]-4-oxo-,
1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 6 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN

REFERENCE COUNT:

THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 6 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN

249540-84-9 CAPLUS
Pentanoic acid, 5-[[(1,1-dimethylethoxy)carbonyl][[((15,4R)-7,7-dimethyl-2-oxobicyclo[2,2,1]hept-1-yl]methyl]sulfonyl]amino]-3-[((25)-4-(1,1-dimethylethoxy)-2-(1-methylethyl)-1,4-dioxobutyl]amino]-4-oxo-,phenylmethyl ester (9C1) (CA INDEX NAME)

Absolute stereochemistry.

249540-85-0 CAPLUS
Pentanoic acid, 5-[[[[15,4R]-7,7-dimethyl-2-oxobicyclo[2.2.1]hept-1-yl]methyl]sulfonyl]amino]-3-[[(25)-2-(1-methylethyl)-1,4-dioxo-4-[(phenylmethoxy)amino]butyl]amino]-4-oxo-, phenylmethyl ester (9CI) (CA INDEX NAME)

L7 ANSWER 7 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER:
1999:670116 CAPLUS
131:295568
C- and R-Amino acid hydroxyethylamino
sulfonamides useful as retroviral protease inhibitors
Vazques, Michael L., Mueller, Richard A.; Talley, John
J.; Getman, Daniel P.; Decrescenzo, Gary A.; Freskos,
John N.; Bertenshaw, Deborah E.; Heintz, Robert M.
G. D. Searle and Co., USA
COOEN: USXCAM
DOCUMENT TYPE:
LANGUAGE:
FAMILY ACC. NUM. COUNT:
PATENT INFORMATION:
English
FAMILY ACC. NUM. COUNT:
PATENT INFORMATION:

FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

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		6924				B1		2005	0802		US 2	003-	6333	76		2	0030	804	
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											US 1	994-	2944	68		A1 1	9940	823	
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US 18797-2880UN Al 19990408

US 2001-798255 Al 20010305

US 2002-157019 Al 20010305

US 2002-157019 Al 20020530

U OTHER SOURCE(S):

ANSYER 7 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN (Continued) 159005-89-7 CAPLUS Butanedianide, NI-[(15,2R)-2-hydroxy-3-[(3-methylbutyl) (methylsulfonyl) amino]-1-[phenylmethyl) propyl]-2-[(2-quinolinylcarbonyl) amino]-, (25)- (9CI) (CA INDEX NAME)

## Absolute stereochemistry.

159005-90-0 CAPLUS
2-Thia-3,7,10-triazaundecan-11-oic acid, 9-(2-amino-2-oxoethyl)-5-hydroxy-3-(3-methylbutyl)-8-oxo-6-(phenylmethyl)-, phenylmethyl ester, 2,2-dioxide, (5%,6%,9%)- (9CI) (CA INDEX NAME)

#### Absolute stereochemistry.

159005-91-1 CAPLUS Butanediamide, NI-{(15,2R)-2-hydroxy-3-{(3-methylbutyl)(phenylsulfonyl)amino]-1-(phenylsethyl)propyl}-2-{(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

## Absolute stereochemistry.

ANSWER 7 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
as retroviral protease inhibitors)
15906-21-0 CAPLUS
Carbamic acid, {[15]-3-amino-1-[[[[15,2R]-2-hydroxy-1-(phenylmethyl)-3-[[phenylaulfonyl)]-propylamino]propyl]amino]carbonyl]-3-oxopropyl]-,
phenylmethyl ester (9CI) (CA INDEX NAME)

159006-22-1 CAPLUS
Cacbamic actd, [(15)-1-[[[(15,2R)-2-hydroxy-3-[(3-mathylbutyl) (phenylsulfonyl) amino]-1-(phenylmethyl) propyl] amino]carbonyl]-3-(aethylamino)-3-oxopropyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

# Absolute stereochemistry.

REFERENCE COUNT:

THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 7 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN

159005-92-2 CAPLUS
Carbanic acid, [(15)-3-amino-1-[[[(15,2R)-2-hydroxy-3-[(3-methylbutyl) (phenylsulfonyl)amino]-1-[phenylmethyl)propyl]amino]carbonyl]-3-oxopropyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

#### Absolute stereochemistry.

159005-95-5 CAPLUS Butanediamide, NI-{(15,2R)-2-hydroxy-3-[(3-methylbutyl)(phenylsulfonyl)amino]-1-(phenylmethyl)propyl)-N4-methyl-2-[(2-quinolinylcarbonyl)amino]-, (2S)-(9CI) (CA INDEX NAME)

### Absolute stereochemistry.

159006-21-0P 159006-22-1P RL: RCT (Reactant): SPN (Synthetic preparation): PREP (Preparation): RACT (Reactant or reagent) ( $\alpha$ - and  $\beta$ -amino acid hydroxyethylamino sulfonamides useful

L7 ANSWER 8 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER:
1998:799692 CAPLUS
130:38712
1TITLE: Preparation of α- and β-amino acid
hydroxyethylamino sulfonamides useful as retroviral
protease inhibitors
Vazquez, Michael L., Mueller, Richard A., Talley, John
J., Getman, Daniel, Decrescenzo, Gary A., Freskos,
John N.

PATENT ASSIGNEE(S): SOURCE:

John Name, beneath becasened, day An Italian, John Name, and Co., USA
U.S., 67 pp., Cont.-in-part of U.S. Ser. No. 934,984, abandoned.
COUDEN: USKKAM

DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM, COUNT: PATENT INFORMATION.

PATENT	INFORM				•													
PA'	TENT N	o.			KIN	D	DATE			APP	LICAT	NOI	NO.		D.	ATE		
115	58439 81020 81020 81020	46			Δ.		1998	1201		IIS .	1993.	1109	11		11	9930	R24	
170	91020	•			12		1997	1201		ED .	1993-	1134	34		1	9930	R24	
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EP	94766 71561 71561	В			B1		1998	1216										
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AT	17458	7 .			E		1999	0115		AT	1994	9271	62		1	9940	823	
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FI	95006	50			A		1995	0214		FI	1995-	-650			1	9950	214	
FI	11247	1			B1		2003	1215										
US	57864	83			A		1998	0728		US	1995-	4876	62		1	9950	607	
US	58308	97			A		1998	1103		US	1995-	4736	98		1	9950	607	
US	61720	82			B1		2001	0109		US	1995-	4767	88		1	9950	607	
US	57444	81			Α		1998	0428		US	1997-	-8453	92		1	9970	425	
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บร	20020	523	99		A1		2002	0502		US	2001-	-7982	55		2	0010	305	
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AT ESS FI US	20031	913	19		A1		2003	1009		US	2002-	-1570	19		2	0020	530	
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US	69242	86			В1		2005	0802		US	2003-	-6333	76		2	0030	804	
PRIORIT	Y APPL	Ν. :	info	.:						US	1992-	-9349	84		B2 1	9920	825	
										EΡ	1993-	9237	14		A3 1	9930	824	
										US	2003- 1992- 1993- 1993-	-1109	11		A 1	9930	824	

US 1999-288080 Al 19990408
US 2001-798255 Al 20010308
US 2002-157019 Al 2002050
OTHER SOURCE(S): MARPAT 130:38712

AB Amino acid hydroxyethylamino sulfonamide compds. PINECHR2CH(OH)CH2NR3SO2R4
[Pl = alkoxycarbonyl, aralkoxycarbonyl, alkanoyl, cycloalkylachoryl,
cycloalkylalkoxycarbonyl, cycloalkylalkanoyl, aralkanoyl, aroyl,
aryloxycarbonyl, heterocyclylacrbonyl, heterocyclyloxycarbonyl,
heterocyclylalkoxycarbonyl, heterocyclyloxycarbonyl,
heterocyclylalkoxycarbonyl, heterocyclyloxycarbonyl,
heterocyclylalkoxycarbonyl, heterocyclyloxycarbonyl,
heterocyclylalkyl, aryl, cycloalkylalkyl, cycloalkylalkyl,
alkoxyalkyl, cycloalkyl, aryl, cycloalkylalkyl, heterocyclyl, heterocyclylalkyl,
alkoxyalkyl, cycloalkyl, reploalkylalkyl, heterocyclyl, heterocycly,
alkonyl, alkynyl, cycloalkyl, heterocycloalkyl, heterocycly, aryl, aralkyl,
were preparation as retrovical processe inhibitors. Thus,
N-[2R-hydroxy-3-[(4methoxyphenyl)sulfonyl](2-methylpropyl) mino]-15-[phenylmethyl)propyl]-4pyridinecarboxamide was prepared by amidation of isonicotinoyl chloride
hydrochloride with 2R-hydroxy-3-[(2-methylpropyl)](14methoxyphenyl)sulfonyl]amino]-15-(phenylmethyl)propylamine. Protease
inhibitory data are tabulated.
IT 159005-98-7P 159006-21-0P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological
study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
BIOL (Biological study); PREP (Preparation); USES (Uses)
[preparation of amino acid hydroxyethylamino sulfonamides useful as
retroviral protease inhibitors)

RN 159005-99-7 CAPIUS

RN Hanediamide, N1-[(15,2R)-2-hydroxy-3-[(3-methylbutyl) (methylsulfonyl) ami
no]-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl) amino]-, (25)- (9CI)
(CA INDEX NAME)

#### Absolute stereochemistry.

159005-91-1 CAPLUS Butanediamide, N1-{(15,2R)-2-hydroxy-3-{(3-methylbutyl) (phenylsulfonyl) ami no]-1-(phenylmethyl) propyl]-2-{(2-quinolinylcarbonyl) amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

#### L7 ANSWER 8 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

Absolute stereochemistry.

159005-90-0P 159006-05-0P 159006-06-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of amino acid hydroxyethylamino sulfonamides useful as retroviral protease inhibitors)
159005-90-0 CAPLUS
2-Thia-3,7,10-triazaundecan-11-oic acid, 9-(2-amino-2-oxoethyl)-5-hydroxy-3-(3-methylbutyl)-8-oxo-6-(phenylmethyl)-, phenylmethyl ester, 2,2-dioxide, (SR,6S,9S)- (9CI) (CA INDEX NAME)

## Absolute stereochemistry.

159006-05-0 CAPLUS
Butanediamide, 2-amino-N1-[(1S,2R)-2-hydroxy-3-[{3-methylbutyl} (methylbulfonyl) amino]-1-(phenylmethyl)propyl]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L7 ANSWER 8 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

159005-92-2 CAPLUS
Carbamic acid, [(15)-3-amino-1-[([(15,2R)-2-hydroxy-3-{(3-methylbutyl) [henylsulfonyl) amino]-1-(phenylmethyl) propyl]amino] carbonyl]-3-exepropyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

### Absolute stereochemistry.

159005-95-5 CAPLUS Butanediamide, NI-[(15,2R)-2-hydroxy-3-[(3-methylbutyl)(phenylsulfonyl)amino]-1-(phenylsethyl)propyl]-N4-methyl-2-[(2-quinolinylcarbonyl)amino]-, (25)- (9CI) (CA INDEX NAME)

#### Absolute stereochemistry.

159006-21-0 CAPLUS
Carbanic acid, {(15)-3-amino-1-[[[(15,2R)-2-hydroxy-1-(phenylmethyl)-3-[(phenylmylfonyl)propylamino]propyl]amino]carbonyl]-3-oxopropyl]-,
phenylmethyl ester (9CI) (CA INDEX NAME)

#### ANSWER 8 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

159006-06-1 CAPLUS
Butanediamide, 2-amino-N1-[(15,2R)-2-hydroxy-3-[(3-methylbutyl)(phenylsulfonyl)amino]-1-(phenylmethyl)propyl]-, (25)- (9CI)(CA INDEX NAME)

# Absolute stereochemistry

•

REFERENCE COUNT:

THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSVER 9 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1998:502547 CAPLUS
DOCUMENT NUMBER: 129:136097
TITLE: Preparation of heterocyclic sulfonamide inhibitors of

aspactyl protease
Tung, Roger D., Murcko, Mark A., Bhisetti, Govinda Rao
Vertex Pharmaceuticals, Incorporated, USA
U.S., 87 pp., Cont.-in-part of U.S. 5,585,397.
CODEN: USCKAM INVENTOR (5): PATENT ASSIGNEE (5):

DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION: Patent English 5

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5783701	A	19980721	US 1995-393460	19950223
EP 885887	A2	19981223	EP 1998-113921	19930907
EP 885887	A3	19990203		
EP 885887	B1	20030528		
			GB, GR, IT, LI, LU, 1	II. SE. MC. PT. IE
us 5585397	λ		US 1993-142327	
us 5723490	Ä	19980303		
us 5977137	Ä	19991102		
US 6392046	B1	20020521	US 1999-409808	
US 2003064977		20020321	US 2002-94763	20020308
US 6720335	B2		US 2002-94763	20020308
		20040413		
US 2004167116	A1	20040826	US 2004-786997	
PRIORITY APPLN. INFO.:			US 1992-941982	
			US 1993-142327	A2 19931124
			EP 1993-921428	A3 19930907
			WO 1993-US8458	W 19930907
			US 1995-393460	
			US 1998-115394	
			US 1999-409808	
			US 2002-94763	A1 20020308
OTHER SOURCE(S):	MARPAT	129:13609	7	

$$0 \xrightarrow{\begin{array}{c} 0 \\ 0 \end{array}} \stackrel{OH}{\underset{Ph}{\overset{Bu-1}{\bigvee}}} \stackrel{OH}{\underset{0}{\overset{U}{\underset{0}{\bigvee}}}} \stackrel{OH}{\underset{0}{\overset{U}{\underset{0}{\overset{U}{\underset{0}{\bigvee}}}}} \stackrel{OH}{\underset{0}{\overset{U}{\underset{0}{\overset{U}{\underset{0}{\bigvee}}}}} \stackrel{OH}{\underset{0}{\overset{U}{\underset{0}{\overset{U}{\underset{0}{\bigvee}}}}} \stackrel{OH}{\underset{0}{\overset{U}{\underset{0}{\overset{U}{\underset{0}{\overset{U}{\underset{0}{\bigvee}}}}}} \stackrel{OH}{\underset{0}{\overset{U}{\underset{0}{\overset$$

The title compds. I {A = H, -Ht, -R1Ht, (un) substituted -R1-alk(en)ylr R1 = CO, SO2, COCO, OCO, OCO, NR2SO2, NR2CO, NR2COCO; Ht = (un) substituted

ANSVER 9 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
160230-05-79 160230-06-89 160230-07-99
160230-08-09 160230-09-19 160230-10-69
160230-13-99 160230-12-69 160230-13-79
160230-13-99 160230-13-99 160230-27-19
160230-13-79 160230-23-99 160230-23-99
160230-24-09 160230-30-2-69 160230-33-69
160230-24-09 160230-30-2-69 160230-33-69
160231-69-699 160333-42-69 160333-43-79
160333-44-69 160333-42-69 160333-43-79
160333-44-69 160333-45-99
160230-05-69 160333-45-99
160230-05-07 (Bological activity or effector, except adverse); BSU (Biological activity, unclassified); SFN (Synthetic preparation); THU (Therapeutic use);
1010 (Biological study); PREP (Preparation); USES (Uses)
(preparation of heterocyclic sulfonamide derivs. as inhibitors of HIV asparty) protease)
160230-05-7 CAPLUS
Sutanediamide, NI-(1S, 2R)-2-hydroxy-1-(phenylmethyl)-3((phenylmethyl) (phenylsulfonyl) aminol propyl]-2-((2quinolinylcarbonyl) aminol-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

160230-06-8 CAPLUS
Butanediamide, N1-((15,2R)-3-[[[3-(acetylamino)-4fluorophemyl]sulfonyl](phenylmethyl)amino]-2-hydroxy-1(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA
INDEX NAME)

Absolute stereochemistry.

160230-07-9 CAPLUS
Butanediamide, N1-{(15,2R)-3-[[(3,5-dimethyl-4-isoxazolyl)aulfonyl](phenylmethyl)anino]-2-hydroxy-1-(phenylmethyl)propyl]-2-{(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSVER 9 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN (Continued) cycloalk(en)yl, aryl, (benzo)heterocyclyl: R2 = H, slkyl, -alkyl-R7; B = NAZC(R3)2CO; n = 0, 1; R3 = (un)substituted alk(en)yl or cycloalk(en)yl: n = 1, 2; D, D' = R7, (un)substituted alk(en)yl or cycloalk(en)yl: R7 = (un)substituted alk(en)yl or cycloalk(en)yl: R7 = (un)substituted alk(en)yl or cycloalk(en)yl: R7 = (un)substituted alk(en)yl or carbocyclyl: R4 = OR2, COMENZ, OSZNERZ, halo, NRZCORZ, cyanol are prepd. as inhibitors of HIV aspartyl protease. The invention also relates to pharmaceutical compns. comprising these compds. The compds. and pharmaceutical compns. are particularly well suited for inhibiting HIV-1 and HIV-2 protease activity. The invention also relates to methods for inhibiting the activity of HIV aspartyl protease using the invention compds., and to methods for screening compds. for anti-HIV activity. Prepns. of almost 200 compds. are described, and some of these plus addnl. compds. are claimed. Some of the compds., e.g., iI, inhibit HIV replication (ICSO) in CCMM-CD4 cells in vitro at concns. of \$100 Ml.

18643-21-89

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (intermediate; preparation of heterocyclic sulfonamide derivs. as of HIV aspartyl protease)

inhibitors

of HIV aspartyl protease)

N 186463-21-8 CAPLUS

Sutanediamide, NI-[(15,2R)-3-[[[3-(aminosulfonyl)phenyl]sulfonyl](phenylme thyl)amino]-2-hydroxy-1-[phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)-, mono(trifluoroacetate) (salt) (9CI) (CA INDEX NAME)

CH 1

CRN 160230-14-8 CMF C37 H38 N6 O8 S2

Absolute stereochemistry.

CH

ANSWER 9 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

160230-08-0 CAPLUS
Butanediamide, N1-[(15,2R)-2-hydroxy-1-(phenylmathyl)-3-[(phenylmathyl)[[3-trifluoromethyl)phenyl]sulfonyl]amino]-propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

160230-09-1 CAPLUS Butanediamide, N1-[(15,2R)-3-[[(2-(acetylamino)-4-methyl-5-thiazolyl] sulfonyl] (phenylmethyl) amino]-2-hydroxy-1-(phenylmethyl) propyl]-2-[(2-quinolinylcarbonyl) amino]-, (25)- (9CI) (CA INDEX NAME)

louzablo=10-4 Cartos
Sutanediamide, N1-[(15,2R)-2-hydroxy-3-[[[5-(3-isoxazoly1)-2-thienyl]sulfonyl](phenylmethyl)amino]-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (25)- (9CI) (CA INDEX NAME)

RN 160230-11-5 CAPLUS
CN Benzoic acid, 3-[[[(2R,3\$)-3-[[(2S)-4-amino-1,4-dioxo-2-[(2-quinolinylcarbonyl)amino]butyl]amino]-2-hydroxy-4-phanylbutyl](phenylmethyl)amino]sulfonyl]- (9Cl) (CA INDEX NAME)

Absolute stereochemistry.

RN 160230-12-6 CAPLUS
CN ButanedLamide, Nl-{(15,2R)-2-hydroxy-3-[(methylsulfonyl) (phenylmethyl) amin
o]-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (25)- (9Cl)
(CA INDEX NAME)

Absolute stereochemistry.

RN 160230-13-7 CAPLUS
CN Butanediade, N1-[(1s,2R)-3-[(2,1,3-benzoxadiazol-4ylsulfonyl)(phenylmethyl)aminoj-2-hydroxy-1-(phenylmethyl)propyl]-2-[(2quinolinylcarbonyl)amino]-, (25)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L7 ANSWER 9 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

RN 160230-18-2 CAPLUS
CN Butanediamide, NI-[(15,2R)-3-[[(4-fluorophenyl)sulfonyl](2-methylpropyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 160230-19-3 CAPLUS
CN Butanediamide, N1-[(15,2R)-3-[[[4-(acetylamino)-3-fluorophenyl]sulfonyl](2-methylpropyl)amino]-2-hydroxy-1-(phenylmethyl)propyl)-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Absolute stereochemistry.

L7 ANSWER 9 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN

RN 160230-14-8 CAPLUS
CN Butanediamide, N1-((1s,2R)-3-{[[3-(aminosulfonyl)phenyl]sulfonyl](phenylmethyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2s)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 160230-16-0 CAPLUS
CN Butanediamide, Nl-{(15,2R)-2-hydroxy-3-[(2-methylpropyl)[[5-(2-pyridinyl)-2-thenyl]suffonyl]amino]-1-(phenylmethyl)propyl)-2-[(2-quinolinylcarbonyl)amino]-, (25)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 160230-17-1 CAPLUS
CN Butanedianide, N1-[(1s,2R)-2-hydroxy-3-[(2-methylpropyl)[[4-(phenylsulfonyl)-2-thienyl]sulfonyl]anino]-1-(phenylmethyl)propyl}-2-[(2-quinolinylcarbonyl)amino]-, (25)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

L7 ANSWER 9 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

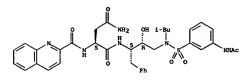
RN 160230-21-7 CAPLUS
CN Butanediamide, N1-[(15,2R)-3-{[(4-(acetylamino)phenyl]sulfonyl]{2methylpropyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-2-[(2quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 160230-22-8 CAPLUS
CN Butanediamide, N1-{(1s,2R)-3-[[[2-(acetylamino)-4-methyl-5-thiao;lyl]sulfonyl}{2-methylpropyl)aminoj-2-hydrosy-1-(phenylmethyl)propyl}-2-[(2-quinolinylcatbonyl)aminoj-, (25)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 160230-23-9 CAPLUS
CN Butanediamide, N1-[(1s,ZR)-3-[[[3-(acetylamino) phenyl] sulfonyl] (2-methylpropyl) amino]-2-hydroxy-1-(phenylmethyl) propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)



160230-24-0 CAPLUS Butanediamide, NI-[(15,2R)-3-[(2,1,3-benzoxadiazol-4-ylsulfonyl) (2-methylpropyl) amino]-2-hydroxy-1-(phenylmethyl)propyl)-2-[(2-quinolinylcarbonyl)amino]-, (25)- (9C1) (CA INDEX NAME)

Absolute stereochemistry.

160230-50-2 CAPLUS
Butanediamide, N-[[15,2R]-3-[[[4-(acetylamino)phenyl]sulfonyl](2-methylpropyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

160231-93-6 CAPLUS Butanediamide, NI-((15,25)-2-hydroxy-3-[[[5-(3-isoxazolyl)-2-thienyl]sulfonyl](2-methyl)propyl)amino]-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (25)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 9 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

160333-44-8 CAPLUS Butanediamide, NI-([15,25)-3-[[4-(acetylamino)phenyl]sulfonyl](2-methylpropyl)amino]-2-hydromy-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (25)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Absolute stereochemistry.

77

RÉFERÈNCE COUNT:

THERE ARE 77 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 9 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN

160231-96-9 CAPLUS
Butanediamide, N1-[(15,2R)-3-[[[4-(acetylamino)-3fluorophenyl]sulfonyl] (phenylmethyl) amino]-2-hydroxy-1(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl) amino]-, (25)- (9CI) (CA
INDEX NAME)

Absolute stereochemistry.

Absolute stereochemistry.

Absolute stereochemistry.

L7 ANSWER 10 OF 19
ACCESSION NUMBER:
1998:501276 CAPLUS
129:170511
1Use of quinoxalines in three-way combinations with protease inhibitors and drug for treating AIDS and/or HIV infections

INVENTOR(S):
PATENT ASSIGNEE(S):
SOURCE:
PATENT ASSIGNEE(S):
SOURCE:
COURT TYPE:
LANGUAGE:
COURT GEVERN
FAMILY ACC. NUM. COUNT:
FAMILY ACC. NUM. COUNT:
CAPLUS COPPRIGHT 2005 ACS on STN
1998:501276 CAPLUS
1099:501276 CAPLUS

DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PRI

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	DE	1970	3131			A1		1998	0730		DE	1997	-1970	3131		1	9970	129
	CA	2278	773			AA		1998	0730		CA	1998	-2278	773		1	9980	115
	WO	9832	442			A1		1998	0730		WO	1998	-EP19	7		•	9980	115
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													ID,					
													, MD,					
													, sk,					
													, KG,					
		RW:	GH,	GM,	KE,	LS,	MW,	SD,	SZ,	UG,	ZW	, AT	BE,	CH,	DE,	DK,	ES,	FI,
			FR,	GB,	GR,	IE,	IT,	LU,	MC,	NL,	PT	, SE	BF,	ВJ,	CF,	CG,	CI,	CM,
			Gλ.	GN.	ML.	MR.	NE.	SN.	TD.	TG								
	AU	9860	940			A1		1998	0818		ΑU	1998	-6094	0		1	9980	115
	ED	9775	70			A1		2000	0209		EP	1998	-9052	97		1	9980	115
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		к.				LV.		55,	,	UD,	0,1	,	,,	20,	,	J.,	,	,
		0007						2000	^221		nn.	1000	-7523			,	0000	115
	BK	9801	523										-7323 -5315					
	JP	2001	5111	24		TZ		2001	0807									
	ZA	9800	679			A		1998	0805				-679					
	NO	9903	670			A		1999	0910		NO	1999	-3670			1	19990	728
	MX	9907	679 670 077			A		2000	0531	1	MΧ	1999	-7077			1	19990	729
0	RIT	Y APE	LN.	INFO	. :						DE	1997	-1970	3131		A 1	19970	129
-													-EP19				9980	

Quinoxaline derivs. in combination with protease inhibitors and reverse transcriptase inhibitors inhibited HIV replication in human lymphocytes. Such 3-way combinations are synergistic and may be used to treat persons with HIV infections or AIDS.

181703-69-5, AN 11686

RL: BAC (Biological activity or effector, except adverse); BFR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)

(AIDS and HIV infections treatment by combinations of quinoxalines and reverse transcriptase inhibitors with protease inhibitors such as); 11703-69-5 CAPLUS

Butanediamide, NI-[(15,2R)-2-hydroxy-3-[(2-methylpropyl) (methylsulfonyl) am ino]-1-(phonylmethyl)propyl]-2-[(2-quinolinylcarbonyl) amino]-, (25)- (9CI) (CA INDEX NAME) AB

ΙŤ

ANSWER 11 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
The title compds. I [A = 3-tetrahydrofuryloxycarbonyl; D' =
(un) substituted alkyl; E = (un) substituted aryl] are prepared This
invention also relates to pharmaceutical compns. comprising these compds.
The compds. and pharmaceutical compns. of this invention are particularly
well suited for inhibiting HIV-1 and HIV-2 protease activity and
consequently, may be advantageously used as antiviral agents against the
HIV-1 and HIV-2 viruses. This invention also relates to methods for
inhibiting the activity of HIV aspartyl protease using the compds. of this
invention and methods for screening compds. for anti-HIV activity. The
title compds. inhibit HIV replication at concentration of ≤ 100 nM.
160230-05-7P 160230-06-8P 160230-10-4P
160230-11-5P 160230-16-0P 160230-13-7P
160230-16-2P 160230-16-0P 160230-13-7P
160230-18-2P 160230-18-3P 160230-22-9P
160230-24-0P 160230-22-2P 160230-23-9P
160230-24-0P 16033-44-6P 160333-44-6P 160333-34-7P
160333-44-6P 160333-45-69 160333-34-7P
180333-44-6P 160333-45-69 160330-30-6P
160230-05-7 CAPIUS
BIOL (Biological study); PREP (Preparation); VEES (Uses)
(preparation of sulfonamide inhibitors of aspartyl protease)
160230-05-7 CAPIUS
Butanediamide, NI-[(15,2R)-2-hydroxy-1-(phenylmethyl)-3[(phenylmethyl) (phenylsulfonyl) amino] propyl]-2-[(2quinolinylcarbonyl) amino]-, (25)- (SCI) (CA INDEX NAME)

## Absolute stereochemistry.

160230-06-8 CAPLUS Butanediamide, N1-([15,2R)-3-[[[3-(acetylamino)-4-fluorophenyl]sulfonyl](phenylmethyl)amino)-2-hydroxy-1-(phenylmethyl)propyl)-2-[(2-quinolinylcarbonyl)amino]-, (25)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L7 ANSVER 11 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1997:9928 CAPLUS
1171LE: 126:144117
Preparation of sulfonamide inhibitors of asparty1
protease

INVENTOR(S): Tung, Roger D.; Murcko, Mark A.; Bhisetti, Govinda R.

Vertex Pharmaceuticals, Incorporated, USA
U.S., 67 pp., Cont. -in-part of U.S. Ser. No.
941,982, abandoned.
CODEN: USKCAM

DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 5

DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PAIENT INFORMATION:			
PATENT NO.	KIND DATE	APPLICATION NO.	DATE
US 5585397	A 19961217	US 1993-142327	19931124
WO 9405639	A1 19940317	US 1993-142327 WO 1993-US8458	19930907
W: AT, AU, BB,	BG, BR, BY, CA,	CH, CZ, DE, DK, ES, I	I, GB, HU, JP,
KP. KR. KZ.	LK. LU. LV. MG.	MN, MW, NL, NO, NZ, I	L. PT. RO. RU.
	UA, US, UZ, VN		
		GB, GR, IE, IT, LU, I	C. NL. PT. SR.
EP 885887	A2 19981223	GN, ML, MR, NE, SN, 1 EP 1998-113921	19930907
EP 885887	A3 19990203		
EP 885887	B1 20030528		
D. AT BY CH	DE DE ES ED	GR GR TT LT LU Y	IL. SE. MC. PT. IE
US 5783701	A 19980721	US 1995-393460	19950223
US 5723490	A 19980303	US 1995-424819	19950419
US 5856353	A 19990105	US 1995-393460 US 1995-424819 US 1995-477937 US 1995-484326 US 1998-115394 US 1998-121008 US 1999-409808	19950607
US 6372778	81 20020416	US 1995-484326 US 1998-115394 US 1998-121008 US 1999-409808 US 2002-94763	19950607
us 5977137	A 19991102	US 1998-115394	19980714
US 6004957	A 19991221	US 1998-121008	19980722
us 6392046	B1 20020521	US 1999-409808	19990930
US 2003064977	A1 20030403	US 2002-94763	20020308
US 6720335			
US 2003069222	A1 20030410	US 2002-94790 US 2004-786997 US 1992-941982 WO 1993-US8458	20020308
US 2004167116		US 2004-786997	20040224
PRIORITY APPLN. INFO.:		US 1992-941982	B2 19920908
		WO 1993-US8458	W 19930907
		EP 1993-921428	A3 19930907
		US 1993-142327	
		US 1995-393460	
		US 1995-484326	
		US 1998-115394	A3 19980714
		US 1999-409808 US 2002-94763	A3 19990930
		us 2002-94763	A1 20020308
comme comments.	WINDS 106-1441		

MARPAT 126:144117

ANSWER 11 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN

160230-07-9 CAPLUS
Butanediamide, N1-[(1s,2R)-3-[(3,5-dimethyl-4isoxazolyl)sulfonyl[(phenylmethyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

## Absolute stereochemistry.

160230-08-0 CAPLUS Butanediamide, N1-[(15,2R)-2-hydroxy-1-(phenylmethyl)-3-[(phenylmethyl)] ([3-trifluoromethyl)phenyl]sulfonyl]amino]propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

## Absolute stereochemistry.

160230-09-1 CAPLUS

100230-09-1 CAZUS
Butanediamide, N1-[(1S,2R)-3-[([2-(acetylamino)-4-methyl-5-thiazolyl]sulfonyl](phenylmethyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

160230-10-4 CAPLUS
Butanediamide, N1-{(15,2R)-2-hydroxy-3-[[[5-(3-isoxazoly1)-2-thieny1] sulfony1](phenylmethy1)amino]-1-(phenylmethy1)propy1]-2-[(2-quinolinylcarbony1)amino]-, (25)- (9CI) (CA INDEX NAME)

#### Absolute stereochemistry.

160230-11-5 CAPLUS
Benzoic acid, 3-{[[(2R,35)-3-{[(2S)-4-amino-1,4-dioxo-2-[(2-quinolinyl(actbonyl) amino]butyl] amino]-2-hydroxy-4-phenylbutyl](phenylmathyl) amino]-ulfonyl]- (9CI) (CA INDEX NAME)

## Absolute stereochemistry.

160230-12-6 CAPLUS Butanediamide, NI-[(15,2R)-2-hydroxy-3-[(methylsulfonyl)(phenylmethyl)amin ol-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

## Absolute stereochemistry.

#### ANSWER 11 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

160230-17-1 CAPLUS
Butanediamide, NI-[(1S,2R)-2-hydroxy-3-{(2-methylpropy1)[[4-(phenylsulfony1)-2-thieny1]sulfony1]amino]-1-(phenylsulfony1)-2-[(2-quinoliny1carbony1)amino]-, (2S)- (9CI) (CA INDEX NAME)

## Absolute stereochemistry.

160230-18-2 CAPLUS
Butanediamide, N1-[(15,2R)-3-[[(4-fluorophenyl)sulfonyl](2-methylpropyl)amino]-2-hydroxy-1-(phenylmethyl)propyl)-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

## Absolute stereochemistry.

160230-19-3 CAPLUS
Butanediamide, N1-[(1S,2R)-3-[[(4-(acetylamino)-3-fluorophenyl]sulfonyl](2-methylropyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

## Absolute stereochemistry.

160230-13-7 CAPLUS
Butanediamide, N1-[(15,2R)-3-[(2,1,3-benzoxadiazol-4ylsulfonyl) (phenylnethyl) amino|-2-hydroxy-1-(phenylnethyl) propyl]-2-[(2quinolinylcarbonyl) amino]-, (25)- (9CI) (CA INDEX NAME)

(Continued)

### Absolute stereochemistry.

160230-14-8 CAPLUS
Butanediamide, NI-[(15,2R)-3-[[[3-(aminosulfonyl)phenyl]sulfonyl](phenylmethyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (25)- (9CI) (CA INDEX NAME)

### Absolute stereochemistry.

 $\label{local-160} \begin{tabular}{ll} 160230-16-0 & CAPLUS \\ Butanediamide, & MI-([15,2R)-2-hydroxy-3-[(2-methylpropyl)[[5-(2-pyridinyl)-2-thionyl]] sulfonyl] aminol-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)aminol-, (2S)- (9CI) & (CA INDEX NAME) \\ \end{tabular}$ 

#### ANSWER 11 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

 $\label{local-20-6} \begin{tabular}{ll} $160230-20-6 & CAPLUS \\ Butanediamide, N1-[[1S,2R]-3-[[[3-(acetylamino)-4-fluorophenyl] sulfonyl] {2-methylpropyl]-2-fluorophenyl] amino]-2-hydroxy-1-(phenylmethyl)propyl]-2-[[2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME) \\ \end{tabular}$ 

## Absolute stereochemistry.

 $\label{local-2-7} \begin{tabular}{ll} 160230-21-7 & CAPLUS & Butanediamide, & M-{(1S,2R)-3-{([4-(acetylamino)phenyl] sulfonyl)} (2-methylpropyl) amino]-2-hydroxy-1-(phenylmethyl)propyl)-2-{(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME) } \end{tabular}$ 

## Absolute stereochemistry.

160230-22-8 CAPLUS Butanediamide, NI-([15,2R]-3-[{[2-(acetylamino)-4-methyl-5-thiazolyl]sulfonyl](2-methylpropyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (25)- [9CI) (CA INDEX NAME)

160230-23-9 CAPLUS Butanediamide, NI-[(1S,2R)-3-[[[3-(acetylamino) phenyl] sulfonyl] (2-methylpropyl) amino]-2-hydroxy-1-(phenylmethyl) propyl]-2-[(2-quinolinylcatbonyl) amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

 $\label{local-24-0} \begin{tabular}{ll} $160230-24-0$ & $CAPLUS$ & $Butanediamide, $N1-\{(1S,2R)-3-\{(2,1,3-benzoxadiazo1-4-ylsulfonyl)(2-methylpropyl)amino]-2-hydroxy-1-\{phenylmethyl)propyl]-2-\{(2-quinolinylcarbonyl)amino]-, $(2S)-(9CI)$ & $(CA INDEX NAME)$ & $(CA$ 

Absolute stereochemistry.

160230-50-2 CAPLUS
Butanediamide, N-[(15,2R)-3-[[[4-(acetylamino)phenyl]sulfonyl](2-methylpropyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 11 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

160333-43-7 CAPLUS Butanediamide, NI-[(15,25)-3-[(2,1,3-benzoxadiazol-4-ylsulfonyl)(2-methylpropyl)amino]-2-hydroxy-1-(phenylmethyl)propyl)-2-[(2-quinolinylcarbonyl)amino]-, (25)- (9CI) (CA INDEX NAME)

160333-44-8 CAPLUS Butanediamide, N1-([15,25]-3-[[[4-(acetylamino)phenyl]sulfonyl](2-methylpropyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (25)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 11 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN

160231-93-6 CAPLUS
Butanediamide, WI-([15,25]-2-hydroxy-3-[[[5-(3-isoxazolyl)-2-thienyl]sulfonyl](2-methylpropyl)amino]-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (25)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

160231-96-9 CAPLUS
Butanediamide, N1-[(15,2R)-3-[[[4-(acetylamino)-3fluocophenyl] suifonyl] (phenylmethyl) aminoj-2-hydroxy-1(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl) aminoj-, (25)- (9CI) (CA
INDEX NAME)

Absolute stereochemistry.

 $\begin{tabular}{ll} 160333-42-6 & CAPLUS \\ Butanediamide, & M-\{(1S,2S)-3-\{[(4-\{acetylamino\}-3-fluorophenyl] sulfonyl](2-methylpropyl) amino]-2-hydroxy-1-\{phenylmethyl)propyl]-2-\{(2-quinolinylcarbonyl) amino]-, (2S)- (9CI) & (CA INDEX NAME) \\ \end{tabular}$ 

Absolute stereochemistry.

ANSWER 11 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

186463-21-8P
RL: RCT (Reactant): SPN (Synthetic preparation): PREP (Preparation): RACT (Reactant or reagent)
(preparation of sulfonamide inhibitors of aspartyl protease)
186463-21-8 CAPUS
Butanediamide, NI-[(1S,2R)-3-[[[3-(aminosulfonyl)phenyl]sulfonyl](phenylme thyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-2-[(2-quinolinyl(arboxyl)amino)-, (2S)-, mono(trifluoroacetate) (salt) (9CI)
(CA INDEX NAME)

CRN 160230-14-9 CMF C37 H38 N6 O8 S2

Absolute stereochemistry.

CM 2

CRN 76-05-1 CMF C2 H F3 O2

L7 ANSWER 12 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1996:601709 CAPLUS
DOCUMENT NUMBER: 125:238651
TITLE: Use of out-out-125:238651
Use of quinoxalines and protease inhibitors in a composition for the treatment of AIDS and/or HIV infections
Paessens, Arnold; Blunck, Martin; Riess, Guenther; Kleim, Joerg-Pater; Roesner, Manfred
Bayer A.-G., Germany
EUr. Pat. Appl., 24 pp.
CODEN: EPXXOW
Patent

INVENTOR(S):

PATENT ASSIGNEE(S): SOURCE:

DOCUMENT TYPE:

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 728481	A2	19960828	EP 1996-102129	19960214
EP 728481	A3	19980708		
R: AT, BE, CH,	, DE, DK	. ES. FR.	GB, GR, IE, IT, LI, LU.	MC. NL. PT. SE
DE 19506742	A1	19960829		19950227
AU 9645615	A1	19960905	AU 1996-45615	19960220
AU 710158	B2	19990916		
CA 2170222	AA	19960828	CA 1996-2170222	19960223
FI 9600850	A	19960828	FI 1996-850	19960223
JP 08245392	A2	19960924	JP 1996-60286	19960223
IL 117247	A1	20001031	IL 1996-117247	19960223
NO 9600775	A	19960828	NO 1996-775	19960226
ZA 9601516	A	19960903	ZA 1996-1516	19960226
BR 9600809	A	19971223	BR 1996-809	19960226
CN 1141196	A	19970129	CN 1996-102709	19960227
PRIORITY APPLN. INFO.:			DE 1995-19506742	A 19950227
OTHER SOURCE(S):	MARPAT	125:2386	51	
GI				
	EP 728481 EP 728481 EP 728481 EP 728481 EP 1506761 DE 19506742 AU 9645615 AU 710158 CA 2170222 FI 9600850 JF 08245392 IL 117247 NO 9600775 ZA 9601516 BR 9600809 CN 1141196 PRIORITY APPLM. INFO.:	EP 728481 A2 EP 728481 A3 EP 728481 A3 EP 728481 A3 EP 328481 A5 DE 19506742 A1 AU 95645615 A1 AU 710158 B2 CA 217022 AA JF 0860850 A JF 08245392 A2 IL 117247 A1 MO 95600775 A ZA 9561516 A BR 9600809 A PRIORITY APPLM. INPO.:  MARPAT	EP 728481 A2 19960828 EP 728481 A3 19980708 R: AT, BE, CH, DE, DK, ES, FM, DE 19506742 A1 19960829 AU 9645615 A1 19960829 AU 710158 B2 19990916 CA 2170222 AA 19960828 JF 0800850 A 19960828 JF 08245392 A2 19960924 JL 117247 A1 20001031 NO 9600775 A 19960828 DF 0808509 A 19971223 CN 1141196 A 19970129 PRIORITY APPLM. INPO.:	EP 728481 A2 19960828 EP 1996-102129 EP 728481 A3 19980708 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, DE 19506742 A1 19960829 DE 1995-19506742 AU 9645615 A1 19960828 AU 1996-45615 AU 710158 B2 19990316 CA 2170222 AA 19960828 C1 1996-2170222 FI 9600850 A 19960828 FI 1996-850 JF 08245392 A2 19960924 JF 1996-650286 IL 117247 A1 20001031 IL 1996-117247 MO 9600775 A 19960828 MO 1996-775 ZA 9601516 A 19960809 A 19970122 A1 1996-11516 BR 9600809 A 19971223 BR 1996-809 CH 141196 PRIORITY APPLM. INFO:  PRIORITY APPLM. INFO:  MARPAT 1251238651

AB Combinations of a quinoxaline derivative [I: R1 - halo, OH, NO2, (substituted)

stituted)

L7 ANSWER 13 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN ACCESSION NUMBER: 1996:47171 CAPLUS DOCUMENT NUMBER: 124:1993129 Determination of the company of the com Determination of protein binding by in vitro charcoal adsorption
Yuan, Jinhua: Yang, Dai Chang: Birkmeier, Jill:

AUTHOR(S):

AUTHOR(5):

Yuan, Jinhua, Yang, Dai Chang, Birkmeier, Jill,
Stolrenbach, James
CORPORATE SOURCE:

Pharmacokinetics, Bioanalytical and Radiochemistry
Function, G. D. Searle Research and Development,
Skokie, IL, 60077, USA

Journal of Pharmacokinetics and Biopharmaceutics
(1995), 23(1), 41-55

CODEN: JPEPBJ ISSN: 0090-466X
Plenum
DOCUMENT TYPE: Journal
LANGUAGE:
English
AB Certain compds. such as SC-52151 have extensive nonspecific adsorption to
the ultrafiltration devices or to dialysis membranes and therefore can not
be measured by the conventional ultrafiltration or equilibrium dialysis
methods. A new method based on charcoal adsorption was developed to
overcome this difficulty. Unlike many conventional methods, which are
based on the separation of free drug from bound drug under equilibrium
conditions,

overcome this difficulty. Unlike many conventional methods, which are based on the separation of free drug from bound drug under equilibrium conditions,
the new method is operated under nonequil. conditions and involves measuring the time course of decline of the percentage of bound drug remaining in plasma while the free drug is being removed by charcoal adsorption. Theor. aspects of the method and the data processing procedure are presented. SC-98A, a compound with minimal nonspecific adsorption to the ultrafiltration membrane, was used to demonstrate the applicability of this method against the ultrafiltration method. Using this method, the protein binding of SC-52151 in human plasma at 1.0 µg/mL was determined to be in the range of 91.4-97.7% at room temperature 157445-98-2, SC 98A
RL: BPR (Biological process); BSU (Biological study, unclassified), THU (Therapeutic use); BIOL (Biological study); PROC (Process); USES (Uses) (protein binding determination by in vitro charcoal adsorption)
RN 157445-98-2 CAPLUS
SUBMANE)

Absolute stereochemistry.

ANSWER 12 OF 19 CAPLUS COPYRIGHT 2005 AC5 on STN (Continued) study, unclassified): THU (Therspeutic use): BIOL (Biological study): USES (Uses)

(Uses)
(use of quinoxalines and protease inhibitors for treatment of AIDS and HIV infections)
181703-69-5 CAPJUS
8utanediamide, N1-[(15,2R)-2-hydroxy-3-[(2-methylpropyl)(methylsulfonyl)amino]-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (23)- [9CI)(CA INDEX NAME)

Absolute stereochemistry.

ACCESSION NUMBER: DOCUMENT NUMBER: TITLE:

INVENTOR(S):

ANSWER 14 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN
SSION NUMBER: 1995:964989 CAPLUS
E: N-[(Succinoylamino)hydroxypropyl]sulfonamides useful
as retroviral protease inhibitors
NTOR(S): Vazquez, Michael L., Hueller, Richard A., Talley, John
J.; Getman, Daniel; Decrescenzo, Gary A.; Freskos,

John N. Searle and Co., USA U.S., 32 pp. Cont.-in-part of U.S. Ser. No. 935,490, abandoned COUDEN: USKKAM PATENT ASSIGNEE (S): SOURCE:

DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION: Patent English

PAIENT INFORMATION:				
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5463104	A	19951031	US 1993-110912	19930824
AT 154800	E	19970715	AT 1993-920213	19930824
ES 2103489	Т3	19970916	ES 1993-920213	19930824
US 5714605	A	19980203	US 1995-541350	19951010
US 5760076	Ä	19980602	US 1995-541747	19951010
US 6022994	Ä	20000208	US 1998-41016	19980312
US 6313345	B1	20011106	US 1999-419816	19991018
US 2002137942	A1	20020926	US 2001-884462	20010620
US 6469207	B2	20021022	00 2001 001102	20010020
US 2003220508	Al	20031127	US 2002-237184	20020909
US 6727282	B2	20040427	03 2002-231104	20020303
US 2005004043	A1	20050106	US 2004-784916	20040224
	W.	20050100		
PRIORITY APPLN. INFO.:				32 19920825
				A3 19930824
			US 1995-541350 A	A1 19951010
			US 1995-541747	A1 19951010
			US 1998-41016	1 19980312
				1 19991018
				1 20010620
				A1 20020909 -
			05 2002-237184	41 20020909 -
OTHER SOURCE(S) .		124 - 176937		

. .

chartylbutyl) (phenylsulfonyl) amino]-1(S)-(phenylmethyl) propyiamine
(preparation
given) followed by benzyl ester hydrogenolysis and amidation, and
exhibited IC50 = 2 nM for inhibition of HHV protease.

I 57448-96-09 157448-97-19 157445-97-19
157445-93-39 157446-00-59 157446-02-19
157446-03-29 157446-07-69 157446-08-49
157446-08-69 157446-07-69 157446-08-79
157446-09-89 157474-44-79 173550-71-19
RL: BAC (Biological activity or effector, except adverse); BSU (Biological
study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
BIOL (Biological study); PREP (Preparation); USES (Uses)

(N-[(succincylamino) hydroxypropyl) sulfonamides useful as retroviral
protease inhibitors)

L7 ANSWER 14 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

157445-99-3 CAPLUS
Butanoic actd, 4-[[2-hydroxy-3-[(2-methylpropyl)(phenylsulfonyl)amino]-1-(phenylmethyl)propyl]amino]-2,2,3-trimethyl-4-oxo-, phenylmethyl ester,
[15-[1R\*(5\*),25\*]]- (9CI) (CA INDEX NAME)

157446-00-9 CAPLUS Butanoic acid, 4-[[2-hydroxy-3-[(2-methylpropyl) (phenylsulfonyl) amino]-1-(phenylmethyl)propyl]amino]-2,2,3-trimethyl-4-oxo-, [IS-[IR\*(S\*),2S\*]]-(9CI) (CA INDEX NAME)

157446-02-1 CAPLUS
Butanoic acid, 4-[[2-hydroxy-3-[[(4-methoxyphenyl)sulfonyl](2-

ANSYER 14 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
157445-96-0 CAPLUS
Butanediamide, N4-[(15,2R)-2-hydroxy-3-{(3-methylbutyl) (phenylsulfonyl) ami
no]-1-(phenylsethyl)propyl)-2,2,3-trimethyl-, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

157445-97-1 CAPLUS Butancic acid, 4-[(2-hydroxy-3-[(3-methylbutyl) (phenylsulfonyl) amino]-1-(phenylmethyl)propyl]amino]-2,2,3-trimethyl-4-oxo-, phenylmethyl ester, [1S-[1R\*(5\*),25\*]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

157445-98-2 CAPLUS Butanotc acid, 4-[(15,2R)-2-hydroxy-3-[(3-methylbutyl) (phenylsulfonyl) amino]-1-(phenylmethyl) propyl] amino]-2,2,3-trimethyl-4-oxo-, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 14 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN (Continued) methylpropyl) amino]-1-(phenylmethyl)propyl] amino]-2,2,3-timethyl-4-oxo-, phenylmethyl ester, [15-[1R(S\*),28\*]]- [9CI) (CA INDEX NAME)

157446-03-2 CAPLUS
Butanoic acid, 4-[(2-hydroxy-3-[((4-methoxyphenyi)sulfonyl](2-methylpropyl)amino]-1-(phenylmethyl)propyl]amino]-2,2,3-trimethyl-4-oxo-,
[15-[18\*(5\*),25\*]]- 9CI) (CA INDEX NAME)

Absolute stereochemistry.

157446-05-4 CAPLUS Butanediamide, N4-[(15,2R)-2-hydroxy-3-[[(4-methoxyphenyl)sulfonyl](3-methylbutyl)amino]-1-(phenylmethyl)propyl]-2,2,3-trimethyl-, (3R)- (9CI)(CA INDEX NAME)

157446-06-5 CAPLUS Butanoic acid, 4-[[2-hydroxy-3-[[(4-methoxyphenyl) sulfonyl)](3-methylbutyl) anino]-1-(phenylmethyl) propyl] anino]-2,2,3-trimethyhenylmethyl ester, [15-[18\*(5\*),25\*]]- (9CI) (CA INDEX NAME) ethvl-4-oxo-.

(Continued)

#### Absolute stereochemistry.

157446-07-6 CAPLUS Butanediamide, N-[(15,2R)-3-[[(4-fluorophenyl)sulfonyl](3-methylburyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-2,2,3-trimethyl-,(3R)- (9CI) (CA INDEX NAME)

## Absolute stereochemistry.

157446-08-7 CAPLUS
Butanotc acid, 4-[[3-[[(4-fluorophenyl)sulfonyl](3-methylbutyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]amino]-2,2,3-trimethyl-4-oxo-, phenylmethyl ester, [1S-[1R\*(S\*),2S\*]]- (9CI) (CA INDEX NAME)

## Absolute stereochemistry.

#### ANSWER 14 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

ANSWER 14 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN

157446-09-8 CAPLUS
Butanoic acid, 4-[[3-[[[4-fluorophenyl]sulfonyl](3-methylbutyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]amino]-2,2,3-trimethyl-4-oxo-,
[15-[1R\*(5\*),25\*]]- (9CI) (CA INDEX NAME)

#### Absolute stereochemistry.

157474-44-7 CAPLUS
Butanoic acid, 4-[[2-hydroxy-3-[[(4-methoxyphenyl) sulfonyl]]3methylbutyl) amino]-1-(phenylmethyl)propyl]amino]-2,2,3-trimethyl-4-oxo-,
[1S-[1R\*(S\*),2S\*]]- (9CI) (CA INDEX NAME)

## Absolute stereochemistry.

173590-71-1 CAPLUS
Butanediamide, W4-([15,2R)-2-hydroxy-3-[(2-methylpropyl)(phenylsulfonyl)aminol-1-(phenylmethyl)propyl]-2,2,3-trimethyl-, (3R)- (9Cl) (CA INDEX

Absolute stereochemistry.

L7 ANSWER 15 OF 19 CAPLUS COPYRIGHT 2005 ACS ON STN ACCESSION NUMBER: 1995:871984 CAPLUS DOCUMENT NUMBER: 123:279761

DOCUMENT NUMBER: TITLE:

INVENTOR(S):

123:279761
Hydroxyethylamino sulfonamides useful as retroviral protease inhibitors
Varquez, Michael L., Mueller, Richard A., Talley, John J., Getman, Daniel P., Decrescenzo, Gary A., Freskos, John N., Bertenshaw, Deborah E., Heintz, Robert M. G.D. Searle and Co., USA) Monsanto Co. PCT Int. Appl., 255 pp.
CODEN: PIXXD2
Patent

PATENT ASSIGNEE(\$): SOURCE:

Patent English

DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PA	TENT	NO.			KIN		DATE					ION			D.	ATE		
¥0	9506	030					1995	0302							1	9940	823	
		AM,																
								KR.										
		NL.	NO.	NZ.	PL.	PT.	RO.	RU,	SD.	SE.	SI.	SK.	TJ.	TT.	UA.	US.	US.	
		UZ,		,	,													
	RW:	KE,		SD.	AT.	BE.	CH.	DE,	DK,	ES,	FR.	GB,	GR,	IE,	IT,	LU,	MC,	
								CG.										TG
US	5843	946			A.		1998	1201		US 1	993-	1109	11		1	9930	824	
US	6060	476			Α		2000	0509		US 1	994-	2048	27		1	9940	302	
AU	9476	697			A1		1995	0321		AU 1	994-	7669	7		1	9940	823	
EP	7156	18			A1		1996	0612		EP 1	994-	9271	62		1	9940	823	
EP	7156	18			B1		1998	1216										
	R:	ΑT,	BE,	CH,														
US	6046	190			A		2000	0404				5868						
PRIORIT	Y APP	LN.	info	.:								1109						
										US 1	994-	2048	27		A 1	9940	302	
												9349						
												US78			A2 1			
												2048						
										WO 1	994-	US91	39		W 1	9940	823	
OTHER S	CITECE	1151 .			MAR	PAT	123:	2797	ผา									

R SOURCE(5): MARPAT 123:279761
Hyrowethylamino sulfonamide compds. AC(1Y)NRGCHR2CHOHCH2NR3S(10)RM4 [1:
Hyrowethylamino sulfonamide compds. AC(1Y)NRGCHR2CHOHCH2NR3S(10)RM4 [1:
R2-(substituted)alkyl, aryl, cycloalkyl, cycloalkylalkyl, aralkyl, R3-H;
R3,R4-R2, alkenyl, alkynyl, heterocycloalkyl, -aralkyl, -aralkyl,
-cycloalkylakyl; R6-H, alkyl; x=1,2; Y=0,5; A-R0, R; R=alkyl, alkenyl;
(hetero)aryl, cycloalkyl, cycloalkylalkyl, aralkyl, NH2, mono- or
disubstituted amino, etc.] are effective as retroviral protease
inhibitors, and in particular as inhibitors of HIV protease. Many
inhibitors were prepared by (1) preparing an N-protected amino epoxide and

inhibitors were prepared by (1) preparing an N-protected amino eposice and ceacting this with an amine and (3) preparing a sulfonamide by reacting with a sulfonyl chloride or sulfonyl anhydride in the presence of an acid scavenger. The amino function of the sulfonamide was then (4) deprotected and (5) reacted with a carboxylate. In vitro HIV protease assays with these compds. revealed inhibitors with ICSO's as low as 1.4 nM, e.g. [15-[1R:9:,2s-1]-1 Ap-HeoCHICHICOCNHCHZCHMe; Y-O; R6-H; RZ-benzyl; R3-3-methylbutyl; x=2; R4-phenyl]. 159006-21-09
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation) (hydroxyethylamino sulfonamides useful as retroviral protease

L7 ANSWER 15 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
inhibitors)
RN 15906-89-7 CAPLUS
Butanedianide, N1-{(15,2R)-2-hydroxy-3-{(3-methylbutyl) (methylsulfonyl) ami
no]-1-(phenylmethyl) propyl]-2-{(2-quinolinylcarbonyl) amino]-, (25)- (9CI)
(CA INDEX NAME)

## Absolute stereochemistry.

159005-91-1 CAPLUS Butanediamide, N1-((15,2R)-2-hydroxy-3-[(3-methylbutyl)(phenylsulfonyl)amino]-1-(phenylmethyl)propyl}-2-[(2-quinolinylcarbonyl)amino]-, (25)- (9CI) (CA INDEX NAME)

#### Absolute stereochemistry.

159005-95-5 CAPLUS Butanediamide, NI-[(1s,2R)-2-hydroxy-3-[(3-methylbutyl) (phenylsulfonyl) ami no]-1-(phenylmethyl)propyl]-N4-methyl-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

## Absolute stereochemistry.

#### ANSWER 15 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

IT

159005-90-0P 159006-03-0P 159006-22-1P
RL: RCT (Reactant): SPN (Synthetic preparation): PREP (Preparation): RACT (Reactant or reagent) (hydroxyethylamino sulfonamides useful as retroviral protease inhibitors)
159005-90-0 CAPLUS
2-Thia-3,7,10-triazaundecan-11-oic acid, 9-(2-amino-2-oxoethyl)-5-hydroxy-3-(3-methylbutyl)-8-oxo-6-(phenylmethyl)-, phenylmethyl ester, 2,2-dioxide, (5R,6S,9S)- (9CI) (CA INDEX NAME)

## Absolute stereochemistry.

159006-05-0 CAPLUS
Butanediamide, 2-amino-N1-[(15,2R)-2-hydroxy-3-[(3-methylbutyl)(methylsulfonyl)amino]-1-(phenylmethyl)propyl]-, (25)- (9CI)(CA INDEX NAME)

## Absolute stereochemistry.

L7 ANSWER 15 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN

159006-21-0 CAPLUS
Carbantc acid, [(15)-3-anino-1-[((15,2R)-2-hydroxy-1-{phenylmethyl}-3-{phenylaulfonyl)propylanino|propyl]anino|carbonyl}-3-oxopropyl}-,
phenylmethyl ester (9CI) (CA INDEX NAME)

## Absolute stereochemistry.

159005-92-2 159006-06-1
RL: RCT (Reactant) r RACT (Reactant or reagent)
(hydrosyethylamino sulfonamides useful as retroviral protease
inhibitors)
159005-92-2 CAPUS
Carbamic acid, [(15)-3-amino-1-[[(15,2R)-2-hydrosy-3-[(3-methylbutyl) (phenylaulfonyl) amino]-1-(phenylmethyl) propyl]amino]carbonyl]3-oxopropyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

## Absolute stereochemistry.

159006-06-1 CAPLUS
Butanediamide, 2-amino-N1-[(15,2R)-2-hydroxy-3-[(3-machlylbutyl) (phenylsulfonyl) amino]-1-(phenylmathyl) propyl]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

# ANSWER 15 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN

159006-22-1 CAPLUS
Carbamic acid, [(15)-1-[[([15,2R)-2-hydroxy-3-[(3-methylbutyl) (phenylsulfonyl) amino]-1-(phenylmethyl) propyl] amino] carbonyl]3-(methylamino)-3-oxopropyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX
NAME)

ACCESSION NUMBER:

DOCUMENT NUMBER: TITLE:

ANSWER 16 OF 19

CAPLUS COPYRIGHT 2005 ACS on STN

ISSION NUMBER:

1995:352211 CAPLUS

122:204547

E: 122:204547

Inhibitors of HIV-1 Protease Containing the Novel and Potent (R)-(Hydroxyethyl) sulfonamide Isostere

Varquez, Nichael L.; Bryant, Martin L.; Clare,
Michaelr DeCrescenzo, Gary A.; Doherty, Elizabeth H.;
Freskos, John N.; Getman, Daniel P.; Houseman, Kathryn
A.; Julien, Janet A.; et al.

ORATE SOURCE: Searle Discovery Research, Skokie, IL, 60077, USA

JOURNAL Of Medicinal Chemistry (1995), 38 (4), 581-4

CODEN: JMCMAR; ISSN: 0022-2623

American Chemical Society

MENT TYPE: AUTHOR (S):

CORPORATE SOURCE: SOURCE:

PUBLI SHER: DOCUMENT TYPE: Journal

LANGUAGE: OTHER SOURCE(5):

MENT TYPE: Journal UNGE: English R SOURCE(S): CASRARCT 122:204547
The authors have prepared and tested a series of novel and highly potent HIV-1 protease inhibitors based on the (R)-(hydroxyethyl) sulfonamide isosters. The isotere exhibits enhanced potency relative to the previously reported (hydroxyethyl)urea isoters. The preferred stereochem. for the critical hydroxyl group is R. X-ray crystallog, studies show that these inhibitors bind to the protease in an extended fashion with one of the sulfonamide oxygens forming a hydrogen bond to the key structural water mol. Some of the compds. showed excellent antiviral activity in vitro.

IT

Water moi: Some Or the company, Short trivitro.

159005-90-0

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)

(inhibitors of HIV-1 protease containing novel and potent

(R) -(hydroxyethyl) sulfonamide isostere in relation to antiviral

(A) -(nydcoyethyl) sultonamude laggetere in relation to antivital activity)

2-filia-3,7,10-triazaundecan-ll-oic acid, 9-(2-amino-2-oxoethyl)-5-hydroxy-3-(3-methylbutyl)-8-oxo-6-(phenylmethyl)-, phenylmethyl ester, 2,2-dioxide, (SA,65,95)- (SCI) (CA INDEX NAME)

#### Absolute stereochemistry.

159005-91-1P
RL: RAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(inhibitors of HIV-1 protease containing novel and potent
(R)-(hydroxyethyl) sulfonamide isostere in relation to antiviral

#### ANSWER 16 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

1.55006-06-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
 (Inhibitors of HIV-1 protease containing novel and potent
 (R)-(hydroxyethyl) sulfonamide isostere in relation to antiviral
 activity)
159006-06-1 CAPLUS
Butanediamide, 2-amino-N1-[(1s, 2R)-2-hydroxy-3-[(3-methylbutyl) (phenylsulfonyl) amino]-1-(phenylmethyl) propyl]-, (2S)- (9CI)
(CA INDEX NAME)

ANSVZR 16 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN (Continued) Butanediamide, N1-[(15,2R)-2-hydroxy-3-[(3-methylbutyl) (phenylsulfonyl) ami no)-1-(phenylsethyl)propyl)-2-[(2-quinolinylcarbonyl)amino]-, (25)- (9CI) (CA INDEX NAME)

## Absolute stereochemistry.

### 159005-89-7P 159005-92-2P

139003-89-FF 139003-92-2F RE: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Usea)

nes) (inhibitors of HIV-1 protease containing novel and potent (R)-(hydroxyethyl)sulfonamide isostere in relation to antiviral

(a) -(hydroxyethyl)sultonamude isostere in texation to antistral activity CAPLUS Butanediamide, Ni-[(15,2R)-2-hydroxy-3-[(3-methylbutyl)(methylsulfonyl)amino]-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (25)- (9CI) (CAINDEX NAME)

#### Absolute stereochemistry.

159005-92-2 CAPLUS
Carbamic acid, ([15)-3-amino-1-[[[(15,2R)-2-hydroxy-3-[(3-methylbutyl) [phenylsulfonyl)amino]-1-[phenylmethyl) propyl]amino]carbonyl]-3-oxopropyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L7 ANSWER 17 OF 19
ACCESSION NUMBER:
DOCUMENT NUMBER:
1171E:
INVENTOR(5):
PATENT ASSIGNEE(5):
SOURCE:
DOCUMENT TYPE:

DOCUMENT TYPE:

CAPLUS COPYRIGHT 2005 ACS on STN
1995:293723 CAPLUS
122:81141
Preparation of heterocyclylarylsulfonamide inhibitors of HIV-aspartyl protease
Tung, Roger D.: Murcko, Mark A.; Bhisetti, Govinda Rao
Vertex Pharmaceuticals Inc., USA
PCT Int. Appl., 291 pp.
COEN: PIXXD2
Patent

DOCUMENT TYPE: LANGUAGE: PAMILY ACC. NUM. COUNT: PATENT INFORMATION:

	PENT				KIN		DATE										ATE	
	9405						1994											
	W:	AT.	AU.	BB.	BG.	BR.	BY.	CA,	CH.	cz	. DI	Ξ,	DK.	ES,	FI,	GB,	HU,	JP,
		KP.	KR.	KZ.	LK.	LU,	LV.	MG,	MN.	MW	. NI	١.	NO.	NZ,	PL.	PT.	RO,	RU,
		SD.	SE.	SK.	UA.	US,	UZ.	VN										
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		BF.	BJ,	CF.	CG.	CI.	CM.	GΑ,	GN.	ML	. MI	R,	NE.	SN.	TD.	TG		
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EP	6591	81			B1		1999	0407										
	D -	3.7	nt	~~	D.C.	O.L.	TC	20	CB	CD			TT	T T	111	MC	MI	27
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ΑU	9348	520			A1		1994	0329										
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FI	9501	059			A		1995	0418		FI	1999	5-:	1059				19950	307
NO	1087 1061 9308 5585 9501 9500 3034	876			A		1995	0508		NO	199	5-6	876				19950	307
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HK	1012	631			A1		2000 2004	0623		HK	199	8-1	1139	71		1	19981	217
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RIT	Y APP	LN.	INFO	- :						US	1993	2-:	9419	82		A2 :	19920	908
										EP	199	3-9	9214	28		A3 :	19930	907
											100			E 0				2002

OTHER SOURCE(S): MARPAT 122:81141

Title compds. A(B) xNECH(D)CH(OR)CH2N(D')SOZE (A = H, Het, R1-Het, (substituted) R1-C1-6 alkyl, (substituted) R1-C2-6 alkenyl wherein R1 = CO, SOZ, COCO, O2C, etc., Het = C5-7 cycloalkyl, C5-7 cycloalkenyl, C6-10 aryl, (substituted) B-7-membered heterocyclyl: R2 = H, (Ar)-C1-3 alkyl: B = NRZCR3CO, null wherein R3 = H, (substituted)Het or C1-6 alkyl or C2-6 alkenyl or C3-6 cycloalkyl or C5-6 cycloalkenyl: x = O, 1: D, D' = Ar, (substituted) C1-6 alkyl wherein R7 = Ph, (substituted) 3-6-membered carbocyclyl or 5-6-membered heterocyclyl: B = Het-O, Het-Het, (substituted) C1-6 alkyl or C2-6 alkenyl, C3-6 carbocyclyl) useful also against viral infection of HIV-2, HIV-2, or HTLV, are prepared 4,3-(AcMH)FCGH3SOCZ1 and syn-1 (A = quinolin-2-ylcarbonyl, D' = Me2CHCH2) (preparation given) in CHZC12 was treated with F3CCO2H followed by NAHCO3 AB

(Continued)

(preparation given) in CH2C12 was treated with F3C0C2H followed by NaHCO3
4-FCGH4SO2C1 to give the title compound II which inhibited HIV-1 protease with ICSO of <0.1 nM.
160230-08-07-79 160230-06-8P 160230-07-9P
160230-08-09 160230-09-1P 160230-10-4P
160230-11-5P 160230-12-6P 160230-13-7P
160230-14-8P 160230-12-6P 160230-21-7P
160230-14-8P 160230-12-9P 160230-22-6P
160230-21-7P 160230-32-8P 160230-22-9P
160230-24-0P 160230-32-8P 160230-32-9P
160230-95-9P 160333-42-6P 160333-43-7P
160333-44-8P 160333-43-9P
RL: SFN (Synthetic preparation); PREF (Preparation)
(preparation of as HIV-1 protease inhibitor)
160230-05-7 CAPLUS
Butanedianide, NI-(IS, ZR)-2-hydroxy-1-(phenylmethyl)-3[(phenylmethyl) (phenylsulfonyl) aminol propyl]-2-((2-quinolinylcarbonyl) aminol-, (2S)- (SCI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 17 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

160230-09-1 CAPLUS
Butanediamide, N1-{(15,2R)-3-{[[2-(acetylamino)-4-methyl-5-thiazolyl]sulfonyl](phenylmethyl)amino]-2-hydroxy-1-(phenylmethyl)propyl}-2-{(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

160230-10-4 CAPLUS
Butanediamide, NI-{(1s,2R)-2-hydroxy-3-[[[5-(3-isoxazoly1)-2-thienyl]sulfonyl](phenylmethyl)amino]-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

160230-11-5 CAPLUS
Benzoic acid, 3-[[(2R,3S)-3-[[(2S)-4-amino-1,4-dioxo-2-[(2-quinolinglizarbonyl)amino]butyl]amino]-2-hydroxy-4phenylbutyl](phenylmethyl)amino]aulfonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

160230-06-8 CAPLUS
Butanediamide, N1-[(1s,2R)-3-[[[3-(acetylamino)-4fluocophenyl] sulfonyl] (phenylmethyl) aminoj-2-hydroxy-1(phenylmethyl) propyl]-2-[(2-quinolinylcarbonyl) aminoj-, (2s)- (9CI) (CA
INDEX NAME)

Absolute stereochemistry.

160230-07-9 CAPLUS
Butanediamide, NI-[(15,2R)-3-[[(3,5-dimethyl)-4-isoxazolyl] gulfonyl] (phenylmethyl) amino]-2-hydroxy-1-(phenylmethyl) propyl]-2-[(2-quinolinylcarbonyl) amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

160230-08-0 CAPLUS
Butanediamide, N1-[(15,2R)-2-hydroxy-1-(phenylmethyl)-3-[(phenylmethyl)[[3-(trifluoromethyl)phenyl]sulfonyl]amino]propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 17 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

160230-12-6 CAPLUS
Butanediamide, NI-{(1S,2R)-2-hydroxy-3-{(methylsulfonyl)(phenylmethyl)amin o]-1-(phenylmethyl)propyl)-2-{(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

160230-13-7 CAPLUS Butanediamide, N1-[(15,2R)-3-[(2,1,3-benzoxadiazol-4-ylsulfonyl) (phenylmethyl) amino]-2-hydroxy-1-(phenylmethyl) propyl]-2-[(2-quinolinylcarbonyl) amino]-, (25)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

160230-14-8 CAPLUS Butanediamide, NI-[(1s,2R)-3-[[[3-(aminosulfonyl)phenyl]sulfonyl](phenylmethyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

RN 160230-16-0 CAPLUS
CN Butanediamide, Nl-{(15,2R}-2-hydroxy-3-{(2-methylpropyl){[5-{2-pyridinyl}-2-thienyl]sulfonyl]amino]-1-(phenylmethyl)propyl}-2-{(2-quinolinylcarbonyl)amino]-, (25)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 160230-17-1 CAPLUS
CN Butanediamide, N1-{(15,2R)-2-hydroxy-3-{(2-methylpropyl){[4-(phenylbulfonyl)-2-thienyl]sulfonyl)amino]-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (25)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 160230-18-2 CAPLUS
CN Butancdianide, N1-[(15,2R)-3-[[(4-fluorophenyl) sulfonyl] (2-sethylpropyl) anino]-2-hydroxy-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (25)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L7 ANSWER 17 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

RN 160230-22-8 CAPIUS
CN Butanediamide, N1-[(15,2R)-3-[[[2-(acetylamino)-4-methyl-5-thiazolyl]yalifonyl](2-methylpropyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (25)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 160230-23-9 CAPLUS
CN Butanediamide, N1-[(15,2R)-3-[[[3-(acetylamino)phenyl]sulfonyl](2-methylpropyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (25)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 160230-24-0 CAPLUS
CN Butanediamide, N1-[(15,2R)-3-[(2,1,3-benzoxadiazol-4-ylsulfonyl) (2-methylpropyl) amino]-2-hydroxy-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (25)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 160230-19-3 CAPLUS

Sutanediamido, N1-[(15,2R)-3-[[[4-(acetylamino)-3-fluorophenyl]sulfonyl](2-methylpropyl)anino]-2-hydroxy-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9C1) (CA INDEX NAME)

Absolute stereochemistry

RN 160230-20-6 CAPLUS

Sutanediamide, N1-[(15,2R)-3-[[[3-(acetylamino)-4-fluorophenyl]sulfomyl](2-methylpropyl)amino]-2-hydroxy-1-(phenylmethyl)propyl)-2-[(2-quinolinylcarbonyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 160230-21-7 CAPLUS
CN Butanediamide, Nl-{(15,2R)-3-[[[4-(acetylamino)phenyl]sulfonyl](2-methylpropyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (25)- (9CI) (CA INDEX NAME)

Absolute stereochemistry

L7 ANSWER 17 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

RN 160230-50-2 CAPLUS
CN Butanediamide, N-[(15,2R)-3-[[[4-(acetylamino)phenyl]sulfonyl](2-methylpropyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 160231-93-6 CAPLUS
CN Butanediamide, N1-{(1s,2s)-2-hydroxy-3-[[[5-(3-isoxazolyl)-2-thienyl]sulfonyl](2-methylpropyl)amino]-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (25)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

## Absolute stereochemistry.

## Absolute stereochemistry.

160333-44-8 CAPLUS Butanediamide, N1-([15,25)-3-[[[4-(acetylamino)phenyl]sulfonyl](2-methylpropyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-, (25)- (9CI) (CA INDEX NAME)

#### Absolute stereochemistry.

L7 ANSWER 18 OF 19 CAP	US COPYRIGHT 2005 ACS on STN								
ACCESSION NUMBER:	994:701324 CAPLUS								
	21:301324								
	Preparation of hydroxyethylamino sulfonamides useful								
	s retroviral protesse inhibitors								
	Vazquez, Michael L.; Mueller, Richard A.; Talley, John								
	.; Getman, Daniel; Decrescenzo, Gary A.; Freskos,								
	ohn N.								
PATENT ASSIGNEE(S):	.D. Searle and Co., USA; Monsanto Co.								
SOURCE:	CT Int. Appl., 198 pp.								
	ODEN: PIXXD2								
	atent								
	nglish								
FAMILY ACC. NUM. COUNT:									
PATENT INFORMATION:									
PATENT NO.	IND DATE APPLICATION NO. DATE								

Pλ	TENT	NO.			KIN	D	DATE			APP	LICAT	ION	NO.		D	ATE	
	9404				λ1	•	1994	0303					14				
	¥:	AT,	AU,	BB,	BG,	BR,	BY,	CA,	Œ,	CZ	, DE,	DK,	ES,	FI.	GB.	HU.	JP.
		KP,	KR,	KZ,	LK,	LU,	MG,	MN,	MV,	NL	, NO,	NZ,	PL,	PT,	RO,	RU,	SD,
			SK,														
	RW:	AT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR	, IE,	IT,	LU,	MC,	NL,	PT,	SE,
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05	2001 2003 6646 2004 6846 6924	1212	19		VI		2003	1009		UŞ	2002-	15/0	19		2	0020	530
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110	2004	2300	22		B1		2005	1110		05	2003-	0333	10		2	0030	804
US	4004	2249	44		A1		∠004	1118		US	2004-	8123	4.5		2	UU40	130

L7 ANSWER 17 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN

160333-45-9 CAPLUS
Butanediamide, N1-{[15,25]-3-{[[3-{acetylamino}-4-fluorophenyl]sulfonyl](2-methylpropyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-2-{[2-quinolinylcarbonyl)amino]-, (25)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L7 ANSWER 18 OF 19 CAPLUS	COPYRIGHT	2005 ACS on STN	(Continued)
PRIORITY APPLN. INFO.:		US 1992-934984	A2 19920825
		EP 1993-923714	A3 19930824
		US 1993-110911	A2 19930824
		WO 1993-US7814	¥ 19930824
		US 1994-204827	A2 19940302
		US 1994-204872	B2 19940302
		US 1994-294468	A1 19940823
		WO 1994-US9139	W 19940823
		US 1995-451090	A3 19950525
		US 1999-288080	A1 19990408
		US 2001-798255	A1 20010305
		us 2002-157019	A1 20020530
		US 2002-199481	A3 20020722

OTHER SOURCE(S): MARPAT 121:301324

AB Title compds. [I and II; R = H, alkoxycarbonyl, aralkoxycarbonyl, alkylcarbonyl, cycloalkylcarbonyl, heterocyclylcarbonyl, heterocycloryalkyl, hydroxyalkyl, aryl, alkyl, alkenyl, alkynyl, substituted aminocarbonyl, etc., R " = H, B3, R "502; RR" = heterocyclyl, heteroaryl; R1 = H, CH2SO2NH2, CH2CO2Me, CO2Me, COMH2, CMe2SH, alkyl, haloalkyl, alkenyl, alkynyl, cycloalkyl, amino acid side chains, etc., R1', R1' = H, R1; 1 of R1', R1' together with R1 form a cycloalkyl radical; R2 = (substituted) alkyl, aryl, cycloalkyl, cycloalkylalkyl, aralkyl; R3 = H, alkyl, haloalkyl, alkenyl, alkenyl, hydroxyalkyl, alkoxyalkyl, cycloalkyl, teterocycloalkyl, heteroaryl, aryl, aralkyl, heteroaralkyl, (substituted) aminoslkyl, etc., R4 = R3, except H; R6 = H, alkyl; x = 0-2; t = 0, 1; Y = 0, S, iminol, were prepared Thus, title compound (III, solution phase preparation given) inhibited HIV protease with ICSO = 16 nH.

IT 159005-89-7P 159005-90-0P 159005-91-IP 159005-92-2P 159005-92-97 159005-92-1P 159005-92-97 159005-95-59 159006-91-1P 159005-92-97 159005-95-59 159006-91-1P 159005-90-91 159005-91-1P 159005-91

ANSWER 18 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN (Continued) study); PREP (Preparation) (prepn. of, as HIV protease inhibitor) (159005-89-7 CAPLUS Butanedianide, NI-([15,2R)-2-hydroxy-3-[(3-methylbutyl) (methylsulfonyl) amino]-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl) amino]-, (25)- (9CI) (CA INDEX NAME)

#### Absolute stereochemistry.

159005-90-0 CAPLUS
2-Thia-3,7.10-triazaundecan-11-oic acid, 9-(2-amino-2-oxoethyl)-5-hydroxy-3-(3-methylbutyl)-8-oxo-6-(phenylmethyl)-, phenylmethyl ester, 2,2-dioxide, (5R,6S,9S)- (9CI) (CA INDEX NAME)

#### Absolute stereochemistry.

159005-91-1 CAPLUS Butanediamide, N1-{(15,2R)-2-hydroxy-3-{(3-methylbutyl) (phenylsulfonyl) amino]-1-(phenylmethyl)propyl]-2-{(2-quinolinylcarbonyl)amino]-, (25)- (9CI) (CA INDEX NAME)

## Absolute stereochemistry.

L7 ANSWER 18 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

## Absolute stereochemistry.

159006-49-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as HIV protease inhibitor intermediate)
159006-49-2 CAPUS
Butanedianide, 2-amino-N1-[2-hydroxy-3-{(3-methylbutyl)| (phenylsulfonyl) amino]-1-(phenylmethyl)propyl]-N4-methyl-, monohydrochloride,
[15-[1R\*(R\*),25\*]]- (9CI) (CA INDEX NAME)

## ● HCl

ΙT

159005-90-0P 159005-92-2P 159006-05-0P
159006-06-1P 159006-22-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as intermediate for HIV protease inhibitor)
159005-90-0 CAPLUS
2-Thia-3,7,10-triazaundecan-11-oic acid, 9-(2-smino-2-oxoethyl)-5-hydroxy-3-(3-sethylbutyl)-8-oxo-6-(phenylmethyl)-, phenylmethyl ester,
2,2-dioxide, (5R,6S,9S)- (9CI) (CA INDEX NAME)

## Absolute stereochemistry.

L7 ANSWER 18 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

159005-92-2 CAPLUS
Carbamic acid, [(15)-3-amino-1-[[((15,2R)-2-hydroxy-3-[(3-methylburyl) [phenylsulfonyl) amino]-1-[phenylmethyl) propyl] amino] carbonyl]-3-oxopropyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

#### Absolute stereochemistry.

159005-95-5 CAPLUS Butanediamide, NI-([15,2R)-2-hydroxy-3-[(3-methylbutyl) (phenylsulfonyl) ami no]-1-(phenylmethyl)propyl]-N4-methyl-2-[(2-quinolinylcarbonyl)amino]-, (25)- (9CI) (CA INDEX NAME)

### Absolute stereochemistry.

159006-21-0 CAPLUS
Carbamic acid, [(15)-3-amino-1-[[[(15,2R)-2-hydroxy-1-(phenylmethyl)-3-[(phenylau/fonyl)propylamino]propyl]amino]carbonyl]-3-oxopropyl}-,
phenylmethyl ester (9CI) (CA INDEX NAME)

#### ANSWER 18 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

159005-92-2 CAPLUS
Carbamic acid, (1(s)-3-amino-1-[[[(1s,2R)-2-hydroxy-3-[(3-methylburly)| phenylaulfonyl) amino]-1-[phenylmethyl) propyl] amino]carbonyl]-3-oxopropyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

## Absolute stereochemistry.

159006-05-0 CAPLUS
Butanediamide, 2-amino-N1-[(1S,2R)-2-hydroxy-3-{(3-methylbutyl) (methylsulfonyl)amino]-1-(phenylmethyl)propyl]-, (2S)- (9CI) (CA INDEX NAME)

159006-06-1 CAPLUS

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ANSWER 18 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
Butanediamide, 2-amino-N1-[(15,2R)-2-hydroxy-3-[(3methylbutyl) (phenylsulfonyl) amino]-1-(phenylmethyl) propyl]-, (25)- (9CI)
(CA INDEX NAME)

Absolute stereochemistry

159006-22-1 CAPLUS
Carbanic acid, [(15)-1-[[([15,2R)-2-hydroxy-3-[(3-methylburly1)[phenylaulfony1]amino]-1-[phenylmethy1)[propy1]amino]carbony1]-3-(methylamino)-3-oxopropy1]-, 1,1-dimethylethy1 ester (9CI) (CA INDEX

Absolute stereochemistry.

ANSWER 19 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN (Continued) = cycloalkyl, aryl, heterocyclyl, etc.; X1 = 0, N, CR17; R17 = H, alkylr Y, Y1 = 0, S, NR15; R15 = H, R3; t = 0, 1; x = 0-2), useful as HIV protease inhibitors for the treatment of A10S, are prepd. Thus, sulfonamide I was prepd. and demonstrated IC50 against HIV protease of 1

sulfoham.de 1 vas prepo. and demonstrated 1.30 against hiv protease of 1 mmol.
137446-05-4 157446-08-6 157474-44-7
RL: RCT (Reactant): RACT (Reactant or reagent)
(HIV protease inhibitor)
157446-05-4 CAPLUS
Butanediam.de, N4-[(1S, 2R)-2-hydroxy-3-([(4-methoxyphenyl)sulfonyl](3-methylbutyl)sulfon-1-(phenylmethyl)propyl]-2,2,3-trimethyl-, (3R)- (9CI)
(CA INDEX NAME)

157446-06-5 CAPLUS
Butanolc acid, 4-[[2-hydroxy-3-[[(4-methoxyphenyl)sulfonyl]]3-methylbutyl]anino]-1-(phenylmethylbyl)anino]-2,2,3-trimethyl-4-oxo-,phenylmethyl ester, [[5-[18\*(5\*),25\*]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

157446-07-6 CAPLUS Butanediamide, Na-[(19,2R)-3-[[(4-fluorophenyl)sulfonyl](3-methylbutyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-2,2,3-trimethyl-,(3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L7 ANSWER 19 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1994:579258 CAPLUS
DICLIMENT NUMBER: 121:179258
H17LE: NUMBER: 179258 N. (alkanoylamino-2-hydroxypropyl) sulfonamides useful as HIV processe inhibitors
Jrycesse inhibitors
Varquez, Michael L.; Mueller, Richard A.; Talley, John J.; Getman, Daniel; Decreacenzo, Gary A.; Freskos, John N.

John N.
G.D. Searle and Co., USA: Monsanto Co.
PCT Int. Appl., 103 pp.
CODEN: PIXXD2
Patent
English
2 PATENT ASSIGNEE(5): SOURCE:

DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PATENT				PINE		DITY			ADE	) T. T C	-2-	I NO I	NO.			DA 7	r		
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WO 940																300	301	200	
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				LK,		MG,	MN,	MV,	NI	., 1	10,	NZ,	PL,	PT.	RQ	, Р	w,	SD,	
				US,															
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	BF,	ВJ,	CF,	œ,	CI,	CH,	GΑ,	GN,	MI	٠, ١	IR,	NB,	SN,	TD,	TG				
EP 656	8886			Al		1995	0614		EP	199	93-9	9202	13			199	301	324	
EP 656	5886			B1		1997	0625												
R	AT.	BE.	CH,	DE.	DK.	ES,	FR,	GB,	GI	1, 1	EE,	IT,	LI,	LU,	NL	, P	т,	SE	
JP 085	00824			T2		1996	0130		JP	199	93-5	5065	31			199	301	924	
AT 154	1800			K		1997	0715		AT	199	93-9	9202	13			199	301	924	
ES 210	3488			T3		1997	0916		ES	199	93-	9202	13			199	30	324	
AU 674	1702			R2		1997	0109		AII	199	33-	5081	9			199	301	125	
AU 93						1994			•••	•••			-						
RU 213						1999	0510		D11	100	35	1068	23			1 99	an:	925	
NO 950									70	100	35.4	67A				100	50	222	
				â		1995			NO.	12:	75-0	243							
FI 950				^		1995	0223												
PRIORITY A	PLN.	INFO	.:										90						
									WO	199	73-l	JS 78	15		w	199	30	825	
OTHER SOURCE	Œ(S):			MARP	'AT	121:	1792	58											
~ 7																			

The title compds. R33(R34)XIC(:Y1)(CH2)tC(R31)(R32)C(R30)(R1)C(:Y)N(R6)C(R2)HC(GH)HCH2N(R3)S(0)RR4 [R1 = H, CH2SO2NH2, COZMe, CONNMe, CONNMe2, etc.; R2 = alkyl, aryl, cycloalkyl, (un)substituted cycloalkylalkyl and arylalkyl; R3 = H, alkyl, haloalkyl, alkenyl, alkynyl, hydroxyalkyl, cycloalkyl, etc.; R4 = alkyl, haloalkyl alkenyl, alkynyl, hydroxyalkyl, alkoxyalkyl, alkoxyalkyl, cycloalkyl, etc.; R4 = alkyl, haloalkyl alkenyl, alkynyl, nydroxyalkyl, alkoxyalkyl, cycloalkyl etc.; R5 = H, alkyl; R30-R32 = R1; R1R30R31 = cycloalkyl; R1R30R32C = cycloalkyl; R33, R34 = H, R3; R33R34X1

ANSWER 19 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN . (Continued)

157446-08-7 CAPLUS Butandc acid, 4-[[3-[[(4-fluorophenyl)sulfonyl](3-methylbutyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]amino]-2,2,3-trimethyl-4-oxo-, phenylmethyl ester, [1S-[1R\*(S\*),2S\*]]- (9CI) (CA INDEX NAME)

157446-09-8 CAPLUS Butanoic acid, 4-[[3-([(4-fluorophenyl)sulfonyl)(3-methylbutyl)amino]-2-hydroxy-1-(phenyliaethyl)propyl]amino]-2,2,3-trimethyl-4-oxo-, [15-[1R\*(5\*),25\*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

157474-44-7 CAPLUS
Butanoic acid, 4-{[2-hydroxy-3-[[(4-methoxyphenyl)sulfonyl](3-methylbutyl)amino]-1-(phenylmethyl)propyl)amino]-2,2,3-trimethyl-4-oxo-,[15-[1R\*(5\*),25\*]]- (9CI) (CA INDEX NAME)

17

157445-96-0P 157445-97-1P 157445-98-2P
157445-99-3P 157446-00-9P 157446-02-1P
157445-03-2P 157446-04-3P
RL: RAC (Biological activity or effector, except adverse): BSU (Biological study, unclassified): SFN (Synthetic preparation): THU (Therapeutic use):
BIOL (Biological study): PREP (Preparation): USES (Uses)
(preparation of, as HIV protease inhibitor)
157445-96-0 CAPLUS
Butanedianide, M4-[1S,2R)-2-hydroxy-3-[(3-methylbutyl) (phenylsulfonyl) ami
no]-1-(phenylmethyl)propyl]-2,2,3-trimethyl-, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

157445-97-1 CAPLUS Butanoic acid, 4-[[2-hydroxy-3-[(3-methylbutyl) (phenylsulfonyl) amino]-1-(phenylmethyl)propyl]amino]-2.2,3-trimethyl-4-oxo-, phenylmethyl ester, [15-[18\*(5\*),25\*]]- [9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWIR 19 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN (Continued) Butanoic acid, 4-{[2-hydroxy-3-[(2-methylpropyl) (phenylsulfonyl) amino]-1-(phenylmethyl)propyl) amino]-2,2,3-trimethyl-4-oxo-, [15-[1R\*(5\*),25\*]]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

157446-02-1 CAPLUS Butanotc acid, 4-[(2-hydroxy-3-[((4-methoxyphenyl) sulfonyl)(2-methylpropyl)amino]-1-(phenylmethyl)propyl)amino]-2,2,3-trimethyl-4-oxo-, phenylmethyl ester, (15-[1R\*(S\*),25\*)]- (9CI) (CA INDEX NAME)

157446-03-2 CAPLUS Butanolc acid, 4-[(2-hydroxy-3-[[(4-methoxyphenyl)sulfonyl](2-methylpropyl)amino]-1-(phenylmethyl)propyl]amino]-2,2,3-trimethyl-4-oxo-,[15-[1R\*(S\*),2S\*]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

157446-04-3 CAPLUS Butanediamide, Na-[[15,2R]-2-hydroxy-3-[[(4-methoxyphenyl)sulfonyl][2-methylpropyl)amino]-1-(phenylmethyl)propyl]-2,2,3-trimethyl-, (3R)- (9CI)(CA INDEX NAME)

L7 ANSWER 19 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN

157445-98-2 CAPLUS Butanoic acid, 4-[(15,2R)-2-hydroxy-3-[(3-methylbutyl)(phenylsulfonyl)amino]-1-(phenylmethyl)propyl]amino]-2,2,3-trimethyl-4-oxo-, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

157445-99-3 CAPLUS Butancic actd, 4-[[2-hydroxy-3-[(2-methylpropyl)(phenylsulfonyl)amino]-1-(phenylmethyl)propyl)amino]-2,2,3-trimethyl-4-oxo-, phenylmethyl ester, [15-[1R\*(5\*),25\*]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

157446-00-9 CAPLUS

L7 ANSWER 19 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN (Continued) Absolute stereochemistry.

=> fil beilstein COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION FULL ESTIMATED COST 95.21 418.94 DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL ENTRY SESSION CA SUBSCRIBER PRICE -13.87-13.87

FILE 'BEILSTEIN' ENTERED AT 18:42:45 ON 11 AUG 2005 COPYRIGHT (c) 2005 Beilstein-Institut zur Foerderung der Chemischen Wissenschaften licensed to Beilstein GmbH and MDL Information Systems GmbH

FILE RELOADED ON OCTOBER 20, 2002 FILE LAST UPDATED ON JUNE 29, 2005

FILE COVERS 1771 TO 2005.
\*\*\* FILE CONTAINS 9,271,550 SUBSTANCES \*\*\*

>>>PLEASE NOTE: Reaction Data and substance data are stored in separate documents and can not be searched together in one query. Reaction data for BEILSTEIN compounds may be displayed immediately with the display codes PRE (preparations) and REA (reactions). A substance answer set retrieved after the search for a chemical name, a compounds with available reaction information by combining with PRE/FA, REA/FA or more generally with RX/FA. The BEILSTEIN Registry Number (BRN) is the link between a BEILSTEIN compound and belonging reactions. For mo detailed reaction searches BRNs can be searched as reaction partner BRNs Reactant BRN (RX.RBRN) or Product BRN (RX.PBRN).<<<

L8 1 SEA SSS SAM L4

=> s L4 full

FULL SEARCH INITIATED 18:42:59 FILE 'BEILSTEIN' FULL SCREEN SEARCH COMPLETED - 164 TO ITERATE

100.0% PROCESSED 164 ITERATIONS

SEARCH TIME: 00.00.07

8 SEA SSS FUL L4

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8 ANSWERS

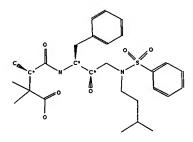
## L9 ANSWER 1 OF 8 BEILSTEIN COPYRIGHT 2005 BEILSTEIN MOL on STN

Beilstein Records (BRN):
Chemical Name (CN):
Autonom Name (AUN):

N-<3-chemzenesulfonyl-(3-methyl-butyl)amino>-1-benzyl-2-hydroxy-propyl>-2,2,3trimethyl-succinamic acid
C28 H40 N2 O6 S
Nolecular Veight (MV):
Lavson Number (LN):
File Segment (FS):
Compound Type (CTYPE):
Constitution ID (CONSID):
Tautomer ID (TAUTID):
Entry Date (DED):
Update Date (DUPD):

Second Very Name (DUPD):

82000/07/18



#### Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
CN	Chemical Name	. 1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	4
FS	File Segment	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
DED	Entry Date	1
DUPD	Update Date	1
PHARM	Pharmacological Data	2

Pharmacological Data:

Results (.RE): binding assay: Contact time 14 min protein binding: Ca. 78 percent Reference(s): 1. Yuan, Jinhuar Yang, Dai Chang: Birkmeier, Jill: Stolzenbach, James, J.Parmacokinet.Biopharm., CODEN: JPBPBJ, 23(1), <1995>, 41 - 56; BABS-6228589

## ANSWER 2 OF 8 BEILSTEIN COPYRIGHT 2005 BEILSTEIN HOL on STN

Beilstein Records (BRN): Chemical Name (CN):

#-(4-<2-(2-amino-3-carbamoyl-propionylamino)-4-<br/>benzenesulfonyl-(3-methyl-butyl)-amino>-3-hydromy-butyl>-

Autonom Name (AUN):

methyl-butyl)-amino>-3-hydromy-butyl>-phenoxy)-butyric acid d-(4-c2-(2-amino)-d-cbenzenesulfonyl-(3-methyl-butyl)-amino>-3-hydromy-butyl>-phenoxy)-butyric acid C29 H42 N4 08 5 606.73 15202, 13803, 3487, 2854, 1789 Steree compound isocvelic

Molec. Formula (MF):
Molecular Weight (MW):
Lawyon Number (LM):
File Segment (FS):
Compound Type (CTYPE):
Constitution ID (CONSID):
Tautomer ID (TAUTIO):
Bellstein Citation (BSO):
Entry Date (DED):
Update Date (DUPD):

isocyclic 6553042 7265790 6-13 1997/07/31 1998/03/04

### Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	5
FS	File Segment	1

- ANSWER 2 OF 8 BELLSTEIN COPYRIGHT 2005 BELLSTEIN HDL on STN Reaction Classification (.CL): Preparation Reagent (.RGT): BOP, DIPEA Reference(s): (Continued)
  - Reference(s):
    1. Abbenarte, G.; Bergman, D. A.; Brinkworth, R. I.; March, D. R.; Reid, R. C.; et al., Bioorg, Med.Chem.Lett., CODEN: BMCLES, 6(21), <1996>, 2531-2536 BABS-6047699

Entry Date Update Date

This substance also occurs in Reaction Documents:

Occurrence Code Reaction Documents Substance is Reaction Reactant Substance is Reaction Product RXREA RXPRO

Reaction: RX

Reaction ID (.ID): Reactant BRN (.RBRN): Reactant (.RCT):

4616107
7446269, 7668064, 1977963
1-bromo-(5)-3-<(tert-butoxycarbonyl)amino>-4-(4'-<3'-carbethoxyrcopyl)oxy>phenyl>-2-butanone, N-(3-eethyl-butyl)-benzenesulfonamides hydrochloride, BOC-L-asparagine 7676992
4-(4-<2-(2-amino-3-carbamoyl-propionylamino)-4-<benzenesulfonyl-(3-methyl-butyl)-amino>-3-hydroxy-butyl>-phenoxy)-butyric acid

Product BRN (.PBRN): Product (.PRO):

No. of React. Details (.NVAR):

Reaction Details:

Reaction RID (.RID): 4616107.1
Reaction Classification (.CL): Preparation
Reagent (.RGT): 1.) DIPEA, 2.) NaBH4, 3.) HCl, 4.) HBTU, DIPEA, 5.) NaOH

Reference(s):
1. Abbenante, G., Bergman, D. A., Brinkworth, R. I., Harch, D. R., Reid, R. C., et al., Bioorg.Med.Chem.Lett., CODEN: BMCLES, 6(21), <1996>, 2531-2536; BABS-6047699

Reaction: RX

Reaction ID (.ID): Reactant BRN (.RBRN): Reactant (.RCT):

4653938
7676982
4-(4-<2-(2-amino-3-carbamoylpropionylamino)-4-<br/>benzeneaulfonyl-(3-amino-3-bydroxy-butyl)-aminoy-3-bydroxy-butyl>phenoxyl-butyric acid<br/>
7676893<br/>2-(11-<2-cbenzenesulfonyl-(3-methyl-butyl)amino>-1-hydroxy-ethyl->-6, 9-dixov-2-oxa-<br/>
7,10-diaza-bicyclo<11.2.2>heptadeca-<br/>
1(16),13(17),14-trien-8-yl)-acetamide Product BRN (.PBRN): Product (.PRO):

No. of React. Details (.NVAR):

Reaction Details:

Reaction RID (.RID): 4653938.1

# ANSWER 3 OF 8 BEILSTEIN COPYRIGHT 2005 BEILSTEIN MDL on STN

Beilstein Records (BRN): Chemical Name (CN):

HT 2005 BELISTEIN MDL on STN

7241722

mino>-1-benzyl-2-hydroxy-propyl>-2(quinoline-2-carbonyl-amino>-uccinamide
N1-<3-<br/>benzenesulfonyl-(3-methyl-butyl)amino>-1-benzyl-2-hydroxy-propyl>-2(quinoline-2-carbonyl)-amino>-succinamide
C35 H41 NS 06 S

659.80
26398, 14921, 13803, 3487, 2854
Stereo compound
heterocyclic
6237125
6902601
6-22
1995/10/31
1996/08/09

Molec. Formula (MF):
Molecular Weight (MW):
Lawson Number (LN):
File Segment (FS):
Compound Type (CTYPE):
Constitution ID (CONSID):
Tautomer ID (TAUTID):
Beilstein Citation (BSO):
Entry Date (DED):
Update Date (DUPD):

# Field Availability:

Code	Name	Occurrence
		***********
BRN	Beilstein Records	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	5
FS	File Segment	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
DED	Entry Date	1
DUPD	Update Date	1
PHARM	Pharmacological Data	1

This substance also occurs in Reaction Documents:

```
ANSVER 3 OF 8 BEILSTEIN COPYRIGHT 2005 BEILSTEIN MDL on STN Code Name Occurrence
Pharmacological Data: PHARM
                                                                     inhibition of recombinant HIV-1 protesse (ICSO 1.5 mM); antiviral activity against the HIVIIB strain of HIV-1 in a CEM cells (ECSO 5 mM)
         Note(s) (.COM):
        Reference(s):
1. Vazquez, Michael L.; Bryant, Martin L.; Clare, Michael; DeCrescenzo, Gary A.; Doherty, Elizabeth M.; et al., J.Med.Chem., CODEN: JMCMAR, 38(4), <1995>, 581-584; BABS-5961570
Reaction:
                                                                     4177267
7236520, 5875502
2-amino-N1-<3-<br/>butyl)-amino>-1-benzyl-2-hydroxy-propyl>-
succinamide, quinoline-2-carboxylic acid
2,5-dioxo-pyrrolidin-1-yl ester
7241722
        Reaction ID (.ID):
Reactant BRN (.RBRN):
Reactant (.RCT):
                                                                    N1-<2-denzenesulfonyl-(3-methyl-butyl) -
amino>-l-benzyl-2-hydroxy-propyl>-2-
<(quinoline-2-carbonyl)-amino>-succinamide
         Product BRN (.PBRN):
Product (.PRO):
         No. of React. Details (.NVAR):
Reaction Details:
        Reaction RID (.RID): 4177267.1
Reaction Classification (.CL): Preparation
```

ANSWER 4 OF 8 BEILSTEIN COPYRIGHT 2005 BEILSTEIN MDL on STN DUPD Update Date PHARM Pharmacological Data

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	2
RXREA	Substance is Reaction Reactant	1
RXPRO	Substance is Reaction Product	1

Pharmacological Data: PHARM Note(#) (.COM):

inhibition of recombinant HIV-1 protease (IC50 2.2 nM)

Reference(s):

1. Vazquez, Michael L.; Bryant, Martin L.; Clare, Michael; DeCrescenzo, Gary A.; Doherty, Elizabeth M.; et al., J.Med.Chem., CODEN: JMCMAR, 38(4), <1995>, 581-584; BABS-5961570

Reaction:

Reaction ID (.ID): Reactant BRN (.RBRN): Reactant (.RCT):

4164071
7225655, 3085452
N-(3-amino-2-hydroxy-4-phenyl-butyl)-N-(3-methyl-butyl)-benzenesulfonamide,
N2-benzyloxycarbonyl-L-asparagine
7241365

Product BRN (.PBRN): Product (.PRO):

No. of React. Details (.NVAR):

Reaction Details:

Reaction RID (.RID): 4164071.1
Reaction Classification (.CL): Preparation
Reagent (.RCT): MBBL, EDC
Solvent (.SOL): dimethylformamide
Reference(s):

1. Vazquez, Michael L.; Bryant, Martin L.; Clare, Michael; DeCrescenzo, Gary A.; Doherty, Elizabeth M.; et al., J.Med.Chem., CODEN: JMCMAR, 38(4), <1995>, 581-584; BABS-5961570

Reaction: RX

Reaction ID (.ID): Reactant ERN (.RERN): Reactant (.RCT):

7241365

(1-<3-<br/>denzenesulfonyl-(3-methyl-butyl)-<br/>amino>-1-benzyl-2-hydroxy-propylcarbamoyl>-<br/>2-carbamoyl-ethyl)-carbamic acid benzyl

ester 7236620 Product BRN (.PBRN): Product (.PRO):

723620 2-amino-N1-<3-<br/>butyl)-amino>-1-benzyl-2-hydroxy-propyl>-succinamide

No. of React. Details (.NVAR):

Reaction Details:

ANSWER 4 OF 8 BEILSTEIN COPYRIGHT 2005 BEILSTEIN MDL on STN

Autonom Name (AUN):

7241365
(1-<3-<br/>
(1-<3-<br/>
(1-<3-<br/>
1-enzyl-2-hydroxy-propylcarbamoyl>2-carbamoyl-ethyl)-carbamic acid benzyl
ester
(1-<3-<br/>
(1-ca)-benzyl-2-hydroxy-propylcarbamoyl>2-carbamoyl-ethyl)-carbamic acid benzyl
ester
(1-<3-<br/>
(1-ca)-benzyl-2-hydroxy-propylcarbamoyl>2-carbamoyl-ethyl)-carbamic acid benzyl
ester

2-carbamoyl-ethyl)-carbamic acid benz ester C33 H42 N4 O7 5 638.78 14921, 13803, 5228, 3487, 2854, 1762 Stereo compound isocyclic 6235878 6895358 6-13 1995/10/31 1996/08/09 Molec. Formula (MF): Molecular Weight (MW): Lawson Number (LM): File Segment (FS): Compound Type (CTYPE): Constitution ID (CONSID): Tautamer ID (TAUTID): Bellstein Citation (BSO): Entry Date (DED):

Entry Date (DED): Update Date (DUPD):

## Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	· Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	6
FS	File Segment	1
CTYPE	Compound Type	1
CONSID	Constitution · ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
DED	Entry Date	1

ANSWER 4 OF 8 BEILSTEIN COPYRIGHT 2005 BEILSTEIN MDL on STN (Continued)

Reaction RID (.RID): 4197780.1
Reaction Classification (.CL): Preparation
Reagent (.RCT): H2
Catalyst (.CAT): 10percent Pd/C
Solvent (.SOL): methanol
Reference(s): 1. Vazquez, Michael L.; Bryant, Martin L.; Clare, Michael; DeCrescenzo,
Gary A.; Doherty, Elizabeth M.; et al., J.Med.Chem., CODEN: JMCHAR,
38 (4), <1995>, 581-584; RABS-5961570

#### ANSWER 5 OF 8 BEILSTEIN COPYRIGHT 2005 BEILSTEIN MOL on STN

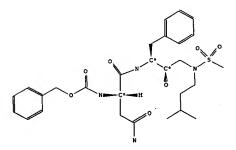
Beilstein Records (BRN): Chemical Name (CN): 7239075
N1-<1-benryl-2-hydroxy-3-<methanesulfonyl(3-methyl-butyl)-amino>-propyl>-2<[quinoline-2-carbonyl)-amino>-succinamide
N1-<1-benzyl-2-hydroxy-3--keethanesulfonyl(3-methyl-butyl)-amino>-propyl>-2<[quinoline-2-carbonyl)-amino>-succinamide
C30 H39 N5 06 S
597.73
26598, 14921, 3487, 2854, 2705
Stereo compound
heterocyclic
6235067
6903688 7239075 Autonom Name (AUN): Molec. Formula (MF):
Molecular Weight (MW):
Lawson Number (LM):
File Segment (FS):
Compound Type (CTYPE):
Constitution ID (CONSID):
Tautomer ID (TAUTIO):
Bellstein Citation (BSO):
Entry Date (DED):
Update Date (DUPD): 6235067 6903688 6-22 1995/10/31

## Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FV	Formular Weight	1
LN	Lawson Number	5
FS	File Segment	1
CTYPE	Compound Type	1
CONSID	Constitution ID	ī
TAUTID	Tautomer ID	· ī
BSO	Beilstein Citation	ī
DED	Entry Date	ī
DUPD	Update Date	ī
PHARM	Pharmacological Data	1

## ANSWER 6 OF 8 BRILSTEIN COPYRIGHT 2005 BRILSTEIN MOL ON STN

Beilstein Records (BRN): Chemical Name (CN): 7238525 (1-<1-benzyl-2-hydroxy-3-<methanesulfonyl-(3-methyl-butyl)-amino>-propylcarbamoyl>-2-carbamoyl-ethyl)-carbamic acid benzyl ester
(1-<1-benzyl-2-hydroxy-3-<methanesulfonyl(3-methyl-butyl)-amino>-propylcarbamoyl>-2carbamoyl-ethyl)-carbamic acid benzyl Autonom Name (AUN): ester C28 H40 N4 07 S Molec. Formula (MF):
Molecular Weight (MW):
Lavson Number (LM):
File Segment (FS):
Compound Type (CTYPE):
Constitution ID (CONSID):
Tautomer ID (TAUTID):
Beilstein Citation (BSO):
Entry Date (DED):
Update Date (DUPD): 576.71 14921, 5228, 3487, 2854, 2705, 1762 Stareo compound isocyclic 6232600 6898701 6-13 1995/10/31 1996/08/09



## Field Availability:

Code	Name	Occurrance
BRN	Beilstein Records	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	6
FS	File Segment	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1

ANSWER 5 OF 8 BEILSTEIN COPYRIGHT 2005 BEILSTEIN MDL on STN This substance also occurs in Reaction Documents:

Reaction Documents Substance is Reaction Product RXPRO

Pharmacological Data: PHARM

Note(s) (.COM):

inhibition of recombinant HIV-1 protease (ICSO 27 nM); antiviral activity against the HIVIIB strain of HIV-1 in a CEM cells (ECSO 53 nM)

(Continued)

Reference(s):

1. Vazquez, Michael L., Bryant, Martin L., Clare, Michael; DeCrescenzo, Gary A., Doherty, Elizabeth M., et al., J.Med.Chem., CODEN: JMCMAR, 38(4), <1995>, 581-584; BABS-5961570

Reaction ID (.ID): Reactant BRN (.RBRN): Reactant (.RCT):

4177266
7230903, 5875502
2-amino-N1-c1-benzyl-2-hydroxy-3cmethanesulfonyl-(3-methyl-butyl)-amino>propyl>-succinamide, quinoline-2carboxylic acid 2,5-dioxo-pyrrolidin-1-yl
seter
7239075
N1-<1-benzyl-2-hydroxy-3-<methanesulfonyl(3-methyl-butyl)-amino>-propyl>-2<(quinoline-2-carbonyl)-amino>-succinamide
1

Product BRN (.PBRN): Product (.PRO):

No. of React. Details (.NVAR):

Reaction Details:

Reaction RID (.RID): 4177266.1
Reaction Classification (.CL): Preparation
Reference(s):
1. Vazquez, Michael L.: Bryant, Martin L.; Clare, Michael; DeCrescenzo,
Gary A.; Doherty, Elizabeth M.: et al., J.Med.Chem., CODEN: JMCMAR,
38(4), <1995>, 581-584; BABS-5961570

(Continued)

ANSWER 6 OF 8 BEILSTEIN COPYRIGHT 2005 BEILSTEIN MDL on STN DED Entry Date 1 Dupd 2005 Date 1 Pharmacological Data 1

This substance also occurs in Reaction Documents:

Code Name Reaction Documents
Substance is Reaction Reactant
Substance is Reaction Product RXREA

Pharmacological Data: PHARM

Note(s) (.COM):

inhibition of recombinant HIV-1 protease (IC50 100 nM)

Reference(s):

1. Vazquez, Michael L., Bryant, Martin L., Clare, Michael, DeCrescenzo, Gary A., Doherty, Elizabeth M., et al., J.Med.Chem., CODEN: JMCMAB, 38(4), <1995>, 581-584; BABS-5961570

Reaction: RX

Reaction ID (.ID): Reactant BRN (.RBRN): Reactant (.RCT):

4164070
7213958, 3085452
N-(3-amino-2-hydroxy-4-phenyl-butyl)-N-(3-methyl-butyl)-methanesulfonamide,
N2-benzyloxycarbonyl-L-asparagine
7238525

Product BRN (.PBRN): Product (.PRO):

7238525 (1-<1-benzyl-2-hydroxy-3-<methanesulfonyl-(3-methyl-butyl)-amino>-propylcarbamoyl>-2-carbamoyl-ethyl)-carbamic acid benzyl

ester 1 No. of React. Details (.NVAR):

Reaction Details:

Reaction RID (.RID): 4164070.1
Reaction Classification (.CL): Preparation
Reagent (.RGT): HDBt, EOC
Solvent (.SOL): dimethylformamide

Reference(s):

1. Vazquez, Michael L., Bryant, Martin L., Clare, Michael, DeCrescenzo, Gary A., Doherty, Elizabeth M., et al., J.Med.Chem., CODEN: JMCMAR, 38(4), <1995>, 581-584; BABS-5961570

Reaction: RX

Reaction ID (.ID): Reactant BRN (.RBRN): Reactant (.RCT): 4197018 7238525

/238525 (1-<1-benzyl-2-hydroxy-3-<methanesulfonyl-(3-methyl-butyl)-amino>-propylcarbamoyl>-2-carbamoyl-ethyl)-carbamic acid benzyl

ester 7230903

Product BRN (.PBRN): Product (.PRO):

2-amino-N1-<1-benzyl-2-hydroxy-3-cmethanesulfomyl-(3-methyl-butyl)-amino>-propyl>-succinamide

No. of React. Details (.NVAR):

L9 ANSWER 6 OF 8 BEILSTEIN COPYRIGHT 2005 BEILSTEIN MDL on STN Reaction Details: RX (Continued)

Reaction RID (.RID): 4197018.1

Reaction Classification (.CL): Preparation
Reagent (.RGT): H2

Catalyst (.CAT): Opercent Pd/C

Solvent (.SOL): methanol

Reference(s): 1. Varquez, Michael L.; Bryant, Martin L.; Clare, Michael; DeCrescenzo,

Gary A.; Doherty, Elizabeth M.; et al., J.Med.Chen., CODEN: JMCHAR,

38(4), <1995>, 581-584; BABS-5961570

Autonom Name (AUN):

Entry Date (DED): Update Date (DUPD):

Beilstein Records (BRN): Chemical Name (CN):

ANSWER 7 OF 8 BEILSTEIN COPYRIGHT 2005 BEILSTEIN MDL on STN

7236620
2-amino-N1-<3-cbenzenesulfonyl-(3-methyl-butyl)-amino-1-benzyl-2-hydroxy-propyl>-succinamide
2-amino-N1-<3-cbenzenesulfonyl-(3-methyl-butyl)-amino-1-benzyl-2-hydroxy-propyl>-succinamide

butyl|-amino>-1-benzyl-2-succinamide C25 H36 N4 O5 S 504.64 14921, 13803, 3487, 2854 5tereo compound isocyclic 6228077 6887578 6-13 1995/10/31 1996/08/09 Molec. Formula (MF):
Molecular Weight (MW):
Lawson Number (LM):
File Segment (FS):
Compound Type (CTYPE):
Constitution ID (CONSID):
Tautomer ID (TAUTION (BSO):
Bellstein Citation (BSO):
Form Name (MFN):

### Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
CN	Chemical Name	1
AUN	Autonomname	1
HF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	4
FS	File Segment	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	i

ANSWER 7 OF 8 BEILSTEIN COPYRIGHT 2005 BEILSTEIN MDL on STN (Continued) DED DUPD Entry Date Update Date

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	2
RXREA	Substance is Reaction Reactant	'1
RXPRO	Substance is Reaction Product	1

Reaction: RX

Reaction ID (.ID): Reactant BRN (.RBRN): Reactant (.RCT):

4197780
7241365
(1-<3-chenzenesulfonyl-(3-methyl-butyl)-amino>-1-benzyl-2-hydroxy-propylcarbamoy2-carbamoyl-ethyl)-carbamic acid benzyl

Product BRN (.PBRN): Product (.PRO):

No. of React. Details (.NVAR):

Reaction Details:

Reaction RID (.RID): 4197780.1
Reaction Classification (.CL): Preparation
Reagent (.RCT): H2
Catalyst (.CAT): 10percent Pd/C
Solvent (.SOL): methanol
Reference(s): 1. Vazquez, Michael L.; Bryant, Martin L.; Clare, Michael; DeGrescenzo,
Gary A.; Doherty, Elizabeth M.; et al., J.Med.Chem., CODEN: JMCHAR,
38(4), <1995>, 581-584; BABS-5961570

Reaction: RX

Reaction ID (.ID):
Reactant BRN (.RBRN):
Reactant (.RCT):
Reactant (.RCT):

Product BRN (.PBRN):
Product (.PRO):
Product (.PRO):

No. of React. Details (.NVAR):

1417267
723620, 5875502
2-amino-N1-<3-chenzenesulfonyl-(3-methyl-butyl)-amino>-1-benzyl-2-hydroxy-propylo-acid 2,5-dioxo-pyrcolidin-1-yl ester 7241722
Nl-<3-chenzenesulfonyl-(3-methyl-butyl)-amino>-1-benzyl-2-hydroxy-propyl>-2<(quinoline-2-carbonyl)-amino>-succinamide

Reaction RID (.RID): 4177267.1
Reaction Classification (.CL): Preparation
Reference(s):
1. Vazquez, Michael L.: Bryant, Nartin L.: Clare, Michael: DeCrescenzo,
Gary A.: Doherty, Elizabeth M.: et al., J.Hed.Chem., CODEN: JNCMAR,
38(4), <1995>, 581-584: BABS-5961570

L9 ANSWER 7 OF 8 BEILSTEIN COPYRIGHT 2005 BEILSTEIN MDL on STN (Continued)

## ANSWER 8 OF 8 BEILSTEIN COPYRIGHT 2005 BEILSTEIN MDL on STN

Beilstein Records (BRN): Chemical Name (CN):

Autonom Name (AUN):

7230903
2-amino-N1-<1-benzyl-2-hydroxy-3cmethanesulfonyl-(3-methyl-butyl)-amino>propyl>-succinamide
2-amino-N1-<1-benzyl-2-hydroxy-3cmethanesulfonyl-(3-methyl-butyl)-amino>propyl>-succinamide
C20 H34 N4 05 5
442.57
14921, 3487, 2854, 2705
Steree compound
isocyclic
6224271
6892172
693172
61395/10/31
1995/10/309

Molec. Formula (MF):
Molecular Weight (MW):
Lavson Number (LN):
File Segment (FS):
Compound Type (CTYPE):
Constitution ID (CONSID):
Tautomer ID (TAUTID):
Bellstein Citation (BSO):
Entry Date (DED):
Update Date (DUPD):

#### Field Availability:

Code	Name	Occurrence
		*************
BRN	Beilstein Records	1
CN	Chemical Name	1
AUN	Autonomname	1
MP	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	4
FS	File Segment	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1.

ANSWER 8 OF 8 BEILSTEIN COPYRIGHT 2005 BEILSTEIN MDL on STN (Continued) ANSWER 8 OF 8 BEILSTEIN COPYRIGHT 2005 BEILSTEIN MDL on STN DED Dupd Entry Date Update Date

This substance also occurs in Reaction Documents:

Code Name Occurrence Reaction Documents Substance is Reaction Reactant Substance is Reaction Product RX RXREA RXPRO

Reaction: RX

Reaction ID (.ID): Reactant BRN (.RBRN): Reactant (.RCT):

4197018
7238525
(1-<1-benzyl-2-hydroxy-3-<methanesulfonyl/3-methyl-butyl)-amino-propylcarbamoyl>-2carbamoyl-ethyl)-carbamic acid benzyl

(Continued)

Product BRN (.PBRN): Product (.PRO): -2-amino-N1-<1-benzy1-2-hydroxy-3-<methanesulfony1-(3-methy1-buty1)-amino>-propy1>-succinamide

No. of React. Details (.NVAR):

Reaction Details: RX

Reaction RID (.RID): 4197018.1
Reaction Classification (.CL): Preparation
Reagent (.RGT): H2
Catalyst (.CAT): 10percent Pd/C
Solvent (.SOL): methanol
Reference(s): 1. Vazquez, Michael L.; Bryant, Martin L.; Clare, Michael DeCrescenzo,
Gary A.; Doherty, Elizabeth M.; et al., J.Med.Chem., CODEN: JMCMAR,
38 (4), <1995>, 581-584; BABS-5961570

Reaction: RX

Reaction ID (.ID): Reactant BRN (.RBRN): Reactant (.RCT):

4177266
7230903, 5875502
2-amino-N1-c1-benzyl-2-hydroxy-3<methanesulfonyl-(3-methyl-butyl)-amino>propyl>-succinamide, quinoline-2carboxylic acid 2,5-dioxo-pyrrolidin-1-yl

Product (.PRO): N1-<1-bezyl-2-hydroxy-3-<methanesulfonyl(3-methyl-butyl)-amino>-propyl>-2<(quinoline-2-carbonyl)-amino>-succinamide

Reaction Details:

Reaction RID (.RID): 4177266.1
Reaction Classification (.CL): Preparation
Reference(s):
1. Vazquez, Michael L.; Bryant, Martin L.; Clare, Michael; DeCrescenzo,
Gary A.; Doherty, Elizabeth M.; et al., J.Med.Chem., CODEN: JMCMAR,
38(4), <1995>, 581-584; BABS-5961570